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☐ 1. Document ID: US 6965850 B2

Using default format because multiple data bases are involved.

L11: Entry 1 of 53 File: USPT Nov 15, 2005

US-PAT-NO: 6965850
DOCUMENT-IDENTIFIER: US 6965850 B2

TITLE: Methods for modulating nuclear receptor coactivator binding

DATE-ISSUED: November 15, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Baxter; John D.	San Francisco	CA		
Darimont; Beatrice	San Francisco	CA		
Feng; Weijun	San Francisco	CA		
Fletterick; Robert J.	San Francisco	CA		
Kushner; Peter J.	San Francisco	CA		
Wagner; Richard L.	San Francisco	CA		
West; Brian L.	San Francisco	CA		
Yamamoto; Keith R.	San Francisco	CA		

US-CL-CURRENT: 703/11; 435/7.1, 702/27, 703/2

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

☐ 2. Document ID: US 6962791 B2

L11: Entry 2 of 53 File: USPT Nov 8, 2005

US-PAT-NO: 6962791
DOCUMENT-IDENTIFIER: US 6962791 B2

TITLE: Treatment or prophylaxis of diseases caused by pilus-forming bacteria

DATE-ISSUED: November 8, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Hultgren; Scott	Ballwin	MO		

Kuehn; Meta	Berkeley	CA	
Xu; Zheng	Blue Bell	PA	
Ogg; Derek	Uppsala		SE
Harris; Mark	Uppsala		SE
Lepisto; Matti	Lund		SE
Jones; Charles Hal	Saint Louis	MO	
Kihlberg; Jan	Dalby		SE

US-CL-CURRENT: 435/7.37; 424/241.1, 424/257.1, 435/849

ABSTRACT:

Novel methods for the treatment and/or prophylaxis of diseases caused by tissue-adhering bacteria are disclosed. By interacting with periplasmic molecular chaperones it is achieved that the assembly of pili is prevented or inhibited and thereby the infectivity of the bacteria is diminished. Also disclosed are methods for screening for drugs as well as methods for the de novo design of such drugs, methods which rely on novel computer drug modelling methods involving an approximative calculation of binding free energy between macromolecules. Finally, novel pyranosides which are believed to be capable of interacting with periplasmic molecular chaperones are also disclosed.

12 Claims, 35 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 25

☐ 3. Document ID: US 6952650 B2

L11: Entry 3 of 53 File: USPT Oct 4, 2005

US-PAT-NO: 6952650
DOCUMENT-IDENTIFIER: US 6952650 B2

TITLE: Modulators of ribosomal function and identification thereof

DATE-ISSUED: October 4, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Steitz; Thomas A.	Branford	CT		
Moore; Peter B.	North Haven	CT		
Ban; Nenad	Zurich			CH
Nissen; Poul	Aarhus N			DK
Hansen; Jeffrey	New Haven	CT		
Ippolito; Joseph A.	Guilford	CT		

US-CL-CURRENT: 702/19; 435/6, 702/20, 702/27

ABSTRACT:

The invention provides methods for producing high resolution crystals of ribosomes and ribosomal subunits as well as crystals produced by such methods. The invention also provides high resolution structures of ribosomal subunits either alone or in combination with protein synthesis inhibitors. The invention provides methods for identifying ribosome-related ligands and methods for designing ligands with specific ribosome-binding properties as well as ligands that may act as protein synthesis inhibitors. Thus, the methods and compositions of the invention may be used to produce ligands that are designed to specifically kill or inhibit the growth of any target organism.

24 Claims, 42 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 36

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw. De

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☐ 4. Document ID: US 6950757 B2

L11: Entry 4 of 53 File: USPT Sep 27, 2005

US-PAT-NO: 6950757
DOCUMENT-IDENTIFIER: US 6950757 B2

TITLE: Screening methods for identifying ligands

DATE-ISSUED: September 27, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Stewart; Lansing J.	Bainbridge Island	WA		

US-CL-CURRENT: 702/27; 117/11, 435/6, 435/7.1

ABSTRACT:

This invention relates to crystallization based assays for identifying ligands that bind to a macromolecule.

5 Claims, 0 Drawing figures
Exemplary Claim Number: 1

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw. De

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☐ 5. Document ID: US 6947845 B2

L11: Entry 5 of 53 File: USPT Sep 20, 2005

US-PAT-NO: 6947845
DOCUMENT-IDENTIFIER: US 6947845 B2

TITLE: Method of identifying molecules that bind to the large ribosomal subunit

DATE-ISSUED: September 20, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Steitz; Thomas A.	Branford	CT		
Moore; Peter B.	North Haven	CT		
Ippolito; Joseph A.	Guilford	CT		
Ban; Nenad	Zurich			CH
Nissen; Poul	Aarhus			DE
Hansen; Jeffrey L.	Charleston	SC		

US-CL-CURRENT: 702/19; 702/20, 702/27

ABSTRACT:

The invention provides methods for producing high resolution crystals of ribosomes and ribosomal subunits as well as crystals produced by such methods. The invention also provides high resolution structures of ribosomal subunits either alone or in combination with protein synthesis inhibitors. The invention provides methods for identifying ribosome-related ligands and methods for designing ligands with specific ribosome-binding properties as well as ligands that may act as protein synthesis inhibitors. Thus, the methods and compositions of the invention may be used to produce ligands that are designed to specifically kill or inhibit the growth of any target organism.

17 Claims, 48 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 42

☐ 6. Document ID: US 6947844 B2

L11: Entry 6 of 53 File: USPT Sep 20, 2005

US-PAT-NO: 6947844
DOCUMENT-IDENTIFIER: US 6947844 B2

TITLE: Modulators of ribosomal function and identification thereof

DATE-ISSUED: September 20, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Steitz; Thomas A.	Branford	CT		
Moore; Peter B.	North Haven	CT		
Ban; Nenad	Zurich			CH
Nissen; Poul	Aarhus N			DK
Hansen; Jeffrey	New Haven	CT		

US-CL-CURRENT: 702/19; 702/27

ABSTRACT:

The invention provides methods for producing high resolution crystals of ribosomes and ribosomal subunits as well as crystals produced by such methods. The invention also provides high resolution structures of ribosomal subunits either alone or in combination with protein synthesis inhibitors. The invention provides methods for identifying ribosome-related ligands and methods for designing ligands with specific ribosome-binding properties as well as ligands that may act as protein synthesis inhibitors. Thus, the methods and compositions of the invention may be used to produce ligands that are designed to specifically kill or inhibit the growth of any target organism.

1 Claims, 42 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 30

☐ 7. Document ID: US 6939848 B2

L11: Entry 7 of 53 File: USPT Sep 6, 2005

US-PAT-NO: 6939848
DOCUMENT-IDENTIFIER: US 6939848 B2

TITLE: Crystals of the large ribosomal subunit

DATE-ISSUED: September 6, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Steitz; Thomas A.	Branford	CT		
Moore; Peter B.	North Haven	CT		
Ban; Nenad	Zurich			CH
Nissen; Poul	Aarhus			DK
Hansen; Jeffrey	New Haven	CT		

US-CL-CURRENT: 514/2; 530/350, 702/19, 702/27

ABSTRACT:

The present invention provides methods for producing high resolution crystals of ribosomes and ribosomal subunits as well as the crystals produced by such methods. The x-ray diffraction patterns of the crystals provided by the present invention are of sufficiently high resolution for determining the three-dimensional structure of ribosomes and ribosomal subunits, for identifying ligand binding sites on ribosomes and ribosomal subunits, and for molecular modeling of ligands which interact with ribosomes and ribosomal subunits. The present invention provides methods for identifying ribosome-related ligands and methods for designing ligands with specific ribosome-binding properties. Thus, the methods of the present invention may be used to produce ligands which are designed to kill or inhibit any

specific target organism(s).

18 Claims, 61 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 23

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. D

☐ 8. Document ID: US 6911528 B1

L11: Entry 8 of 53 File: USPT Jun 28, 2005

US-PAT-NO: 6911528
DOCUMENT-IDENTIFIER: US 6911528 B1

TITLE: Hedgehog-derived polypeptides

DATE-ISSUED: June 28, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Beachy; Philip A.	Baltimore	MD		
Porter; Jeffrey A.	Belmont	MA		

US-CL-CURRENT: 530/350; 530/300, 536/23.5

ABSTRACT:

The present invention provides two novel polypeptides, referred to as the "N" and "C" fragments of hedgehog, or N-terminal and C-terminal fragments, respectively, which are derived after specific cleavage at a G.dwnarw.CF site recognized by the autoproteolytic domain in the native protein. Also included are sterol-modified hedgehog polypeptides and functional fragments thereof. Methods of identifying compositions which affect hedgehog activity based on inhibition of cholesterol modification of hedgehog protein are described.

9 Claims, 132 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 54

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. D

☐ 9. Document ID: US 6889145 B1

L11: Entry 9 of 53 File: USPT May 3, 2005

US-PAT-NO: 6889145
DOCUMENT-IDENTIFIER: US 6889145 B1

TITLE: Three-dimensional model of a Fc region of an IgE antibody and uses thereof

DATE-ISSUED: May 3, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Jardetzky; Theodore S.	Evanston	IL		
Wurzburg; Beth A.	Evanston	IL		

US-CL-CURRENT: 702/27; 703/11

ABSTRACT:

The present invention includes three-dimensional models of antibodies, such as Fc-C.epsilon./C.epsilon.4 regions of IgE antibodies, as well as methods to produce such models. The present invention also includes muteins having increased stability and/or antibody receptor binding activity, as well as methods to produce such muteins, preferably using information derived from three-dimensional models of the present invention. Also included are nucleic acid sequences encoding muteins of the present invention and use of those sequences to produce such muteins. Also included is the use of the model to identify compounds that inhibit the binding of an antibody receptor protein to an antibody. The present invention also includes uses of such muteins and inhibitory compounds, for example, in methods to diagnose and protect animals from allergy and other abnormal immune responses.

11 Claims, 0 Drawing figures
Exemplary Claim Number: 1

☐ 10. Document ID: US 6872542 B1

L11: Entry 10 of 53 File: USPT Mar 29, 2005

US-PAT-NO: 6872542
DOCUMENT-IDENTIFIER: US 6872542 B1

TITLE: Treatment or prophylaxis of diseases caused by pilus-forming bacteria

DATE-ISSUED: March 29, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Hultgren; Scott	Ballwin	MO		
Kuehn; Meta	Berkeley	CA		
Xu; Zheng	Blue Bell	PA		
Ogg; Derek	Uppsala			SE
Harris; Mark	Uppsala			SE
Lepisto; Matti	Lund			SE
Jones; Charles Hal	Saint Louis	MO		
Kihlberg; Jan	Dalby			SE

US-CL-CURRENT: 435/7.32; 424/130.1, 424/164.1, 424/184.1, 424/185.1, 424/234.1,

424/241.1, 424/278.1, 424/9.1, 424/9.2, 435/252.33, 436/501, 530/300, 530/350

ABSTRACT:

Novel methods for the treatment and/or prophylaxis of diseases caused by tissue-adhering bacteria are disclosed. By interacting with periplasmic molecular chaperones it is achieved that the assembly of pili is prevented or inhibited and thereby the infectivity of the bacteria is diminished. Also disclosed are methods for screening for drugs as well as methods for the de novo design of such drugs, methods which rely on novel computer drug modelling methods involving an approximative calculation of binding free energy between macromolecules. Finally, novel pyranosides which are believed to be capable of interacting with periplasmic molecular chaperones are also disclosed.

7 Claims, 35 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 25

☐ 11. Document ID: US 6845328 B2

L11: Entry 11 of 53 File: USPT Jan 18, 2005

US-PAT-NO: 6845328
DOCUMENT-IDENTIFIER: US 6845328 B2

TITLE: Screening methods using the crystal structure of ribosomal protein L11/GTPase activating region rRNA complex

DATE-ISSUED: January 18, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Wimberly; Brian T.	Guilford	CT		
Ramakrishnan; Venkatraman	Salt Lake City	UT		

US-CL-CURRENT: 702/27; 435/7.1, 702/19

ABSTRACT:

The present invention is broadly directed to methods of screening ribosomal protein L11/GTPase activating region (GAR) RNA-modulating compounds by using information from the high-resolution structure of the L11/GAR complex. The methods are useful in identifying compounds useful for anti-bacterial treatments.

6 Claims, 14 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 7

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw. D

☐ 12. Document ID: US 6842704 B2

L11: Entry 12 of 53 File: USPT Jan 11, 2005

US-PAT-NO: 6842704
DOCUMENT-IDENTIFIER: US 6842704 B2

TITLE: Crystalline TNF-.alpha.-converting enzyme and uses thereof

DATE-ISSUED: January 11, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Black; Roy A.	Seattle	WA		
Paxton; Raymond James	Bellevue	WA		
Bode; Wolfram	Gauting			DE
Maskos; Klaus	Holzkirchen			DE
Fernandez-Catalan; Carlos	Martinsried-Planegg			DE
Chen; James Ming	Bedminister	NJ		
Levin; Jeremy Ian	New City	NY		

US-CL-CURRENT: 702/27; 435/15, 435/193, 702/30, 703/1, 703/2

ABSTRACT:

A tumor necrosis factor-.alpha. converting enzyme (TACE) is produced, purified, and crystallized. The three-dimensional coordinates of the crystal are obtained by X-ray diffraction. The coordinates can be recorded on a computer readable medium, or are part of a video memory, where they can be used as part of a system for studying for studying TACE. The coordinates are also used in designing, screening, and developing compounds that associate with TACE.

10 Claims, 7 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 7

☐ 13. Document ID: US 6795776 B1

L11: Entry 13 of 53 File: USPT Sep 21, 2004

US-PAT-NO: 6795776
DOCUMENT-IDENTIFIER: US 6795776 B1

TITLE: Crystallographic structure of the androgen receptor ligand binding domain

DATE-ISSUED: September 21, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Weinmann; Roberto	Lawrenceville	NJ		
Einspahr; Howard M.	Lawrenceville	NJ		
Krystek; Stanley R.	Ringoes	NJ		
Sack; John S.	Lawrenceville	NJ		
Salvati; Mark E.	Lawrenceville	NJ		
Tokarski; John S.	Princeton	NJ		
Attar; Ricardo M.	Lawrenceville	NJ		
Wang; Chihuei	Plainsboro	NJ		

US-CL-CURRENT: 702/27; 530/350, 530/399, 552/621

ABSTRACT:

The first crystal structure of the androgen receptor ligand binding domain has been determined to 2.0 angstrom resolution. Disclosed are the coordinates for the crystal structure, and methods for determining agonists, partial agonists, antagonists, partial antagonists and selective androgen receptors modulators (SARMs) of the androgen receptor.

3 Claims, 4 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 3

☐ 14. Document ID: US 6780975 B2

L11: Entry 14 of 53 File: USPT Aug 24, 2004

US-PAT-NO: 6780975
DOCUMENT-IDENTIFIER: US 6780975 B2

TITLE: Long wavelength engineered fluorescent proteins

DATE-ISSUED: August 24, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Tsien; Roger Y.	La Jolla	CA		
Remington; S. James	Eugene	OR		
Cubitt; Andrew B.	San Diego	CA		
Heim; Roger	Del Mar	CA		
Ormo ; Mats F.	Huddinge			SE

US-CL-CURRENT: 530/350; 536/23.1

ABSTRACT:

Engineered fluorescent proteins, nucleic acids encoding them and methods of use are

provided.

9 Claims, 55 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 53

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

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☐ 15. Document ID: US 6746853 B1

L11: Entry 15 of 53 File: USPT Jun 8, 2004

US-PAT-NO: 6746853
DOCUMENT-IDENTIFIER: US 6746853 B1

TITLE: Proteins with insulin-like activity useful in the treatment of diabetes

DATE-ISSUED: June 8, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Dahiyat; Bassil I.	Los Angeles	CA		
Morton; Andrew G.	late of Mt. Lebanon	PA		

US-CL-CURRENT: 435/69.1; 435/243, 435/320.1, 435/325, 435/69.4, 514/3, 530/303, 536/23.5

ABSTRACT:

The invention relates to novel insulin activity (IA) proteins and nucleic acids. The Invention further relates to the use of the IA proteins in the treatment of insulin related disorders such as type 1 diabetes and type 2 diabetes.

14 Claims, 28 Drawing figures
Exemplary Claim Number: 1,14
Number of Drawing Sheets: 10

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

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☐ 16. Document ID: US 6723710 B2

L11: Entry 16 of 53 File: USPT Apr 20, 2004

US-PAT-NO: 6723710
DOCUMENT-IDENTIFIER: US 6723710 B2

TITLE: Compositions for inhibiting arginase activity

DATE-ISSUED: April 20, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Christianson; David	Media	PA		
Baggio; Ricky	Waltham	MA		
Elbaum; Daniel	Newton	MA		

US-CL-CURRENT: 514/64; 562/7

ABSTRACT:

Compositions and methods for inhibiting arginase activity, including arginase activity in a mammal, are provided. Methods of making the compositions of the invention are also provided as are methods of using the compositions therapeutically. The compositions described herein are useful for alleviating or inhibiting a variety of arinase- and NO synthase-related disorders, including heart disease, gastrointestinal motility disorders, and penile erectile dysfunction in humans.

2 Claims, 49 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 35

☐ 17. Document ID: US 6703486 B2

L11: Entry 17 of 53 File: USPT Mar 9, 2004

US-PAT-NO: 6703486
DOCUMENT-IDENTIFIER: US 6703486 B2

TITLE: Peripheral nervous system specific sodium channels

DATE-ISSUED: March 9, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Mandel; Gail	Stony Brook	NY		
Halegoua; Simon	Belle Terre	NY		
Borden; Laurence A.	Hackensack	NJ		

US-CL-CURRENT: 530/350; 930/10

ABSTRACT:

Cloning, expression, viral and delivery vectors and hosts which contain nucleic acid coding for at least one peripheral nervous system specific (PNS) sodium channel peptide (SCP), isolated PNS SCP, and compounds and compositions and methods, are provided, for isolating, crystallizing, x-ray analysing molecular modeling, rational drug designing, selecting, making and using therapeutic or diagnostic agents or ligands having at least one peripheral nervous system specific (PNS) sodium channel (SC) modulating activity.

5 Claims, 41 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 35

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Drawi D

☐ 18. Document ID: US 6675105 B2

L11: Entry 18 of 53 File: USPT Jan 6, 2004

US-PAT-NO: 6675105
DOCUMENT-IDENTIFIER: US 6675105 B2

TITLE: Structure-based identification of candidate compounds using three dimensional structures and models of Fc receptors

DATE-ISSUED: January 6, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Hogarth; P. Mark	Williamstown			AU
Powell; Maree S.	Ferntree Gully			AU
McKenzie; Ian F. C.	Brunswick			AU
Maxwell; Kelly F.	South Yarra			AU
Garrett; Thomas P. J.	Brunswick			AU
Epa; Vidana	Parkville			AU

US-CL-CURRENT: 702/27; 530/350, 702/19

ABSTRACT:

Disclosed are crystals, crystal structure Fc.gamma.RIIa protein, three dimensional coordinates of Fc.gamma.RIIa protein, and structures and models derived from the Fc.gamma.RIIa structure. Also disclosed are crystals of Fc.epsilon.RI protein and three dimensional coordinates of Fc.epsilon.RI protein monomers and dimers derived from the Fc.gamma.RIIa structure. Also disclosed are three dimensional coordinates of Fc.gamma.RIIIb proteins and models of Fc.gamma.RIIIb derived from the Fc.gamma.RIIa structure. The present invention also includes methods to produce such crystals, crystal structures and models. Uses of such crystals, crystal structures and models are also disclosed, including structure based drug design and therapeutic compositions.

51 Claims, 21 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 18

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Drawi D

☐ 19. Document ID: US 6638908 B1

L11: Entry 19 of 53 File: USPT Oct 28, 2003

US-PAT-NO: 6638908
DOCUMENT-IDENTIFIER: US 6638908 B1

TITLE: Crystals of the large ribosomal subunit

DATE-ISSUED: October 28, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Steitz; Thomas A.	Branford	CT		
Moore; Peter B.	North Haven	CT		
Ban; Nenad	Zurich			CH
Nissen; Poul	Aarhus			DK
Hansen; Jeffrey	New Haven	CT		

US-CL-CURRENT: 514/2; 530/350, 702/19, 702/27

ABSTRACT:

The present invention provides methods for producing high resolution crystals of ribosomes and ribosomal subunits as well as the crystals produced by such methods. The x-ray diffraction patterns of the crystals provided by the present invention are of sufficiently high resolution for determining the three-dimensional structure of ribosomes and ribosomal subunits, for identifying ligand binding sites on ribosomes and ribosomal subunits, and for molecular modeling of ligands which interact with ribosomes and ribosomal subunits. The present invention provides methods for identifying ribosome-related ligands and methods for designing ligands with specific ribosome-binding properties. Thus, the methods of the present invention may be used to produce ligands which are designed to kill or inhibit any specific target organism(s).

28 Claims, 62 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 23

☐ 20. Document ID: US 6631329 B1

L11: Entry 20 of 53 File: USPT Oct 7, 2003

US-PAT-NO: 6631329
DOCUMENT-IDENTIFIER: US 6631329 B1

TITLE: Use of the crystal structure of Staphylococcus aureus isoleucyl-tRNA synthetase in antibiotic design

DATE-ISSUED: October 7, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Wang; Jimin	Hamden	CT		
Silvian; Laura F.	Newton	MA		
Steitz; Thomas A.	Branford	CT		

US-CL-CURRENT: 702/19; 435/193, 435/4, 530/350, 536/23.1, 702/27

ABSTRACT:

The present invention provides the atomic coordinates derived from high resolution x-ray diffraction of the cocrystal complex comprising mupirocin with its target enzyme, isoleucyl-tRNA synthetase from Staphylococcus aureus, and the cognate tRNA.sup.ile from Escherichia coli. The present invention further provides methods of using the atomic coordinates to identify and design new agents which modulate protein synthesis as well as the agents themselves.

23 Claims, 36 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 24

☐ 21. Document ID: US 6596504 B2

L11: Entry 21 of 53 File: USPT Jul 22, 2003

US-PAT-NO: 6596504
DOCUMENT-IDENTIFIER: US 6596504 B2

TITLE: Treatment of prophylaxis of diseases caused by pilus-forming bacteria

DATE-ISSUED: July 22, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Hultgren; Scott	Ballwin	MO		
Kuehn; Meta	Berkeley	CA		
Xu; Zheng	Blue Bell	PA		
Ogg; Derek	Uppsala			SE
Harris; Mark	Uppsala			SE
Lepisto; Matti	Lund			SE
Jones; Charles Hal	Saint Louis	MO		
Kihlberg; Jan	Dalby			SE

US-CL-CURRENT: 435/7.32; 424/130.1, 424/164.1, 424/184.1, 424/185.1, 424/234.1, 424/241.1, 424/278.1, 424/9.1, 424/9.2, 435/252.33, 436/501, 530/300, 530/350

ABSTRACT:

Novel methods for the treatment and/or prophylaxis of diseases caused by tissue-adhering bacteria are disclosed. By interacting with periplasmic molecular

chaperones it is achieved that the assembly of pili is prevented or inhibited and thereby the infectivity of the bacteria is diminished. Also disclosed are methods for screening for drugs as well as methods for the de novo design of such drugs, methods which rely on novel computer drug modelling methods involving an approximative calculation of binding free energy between macromolecules. Finally, novel pyranosides which are believed to be capable of interacting with periplasmic molecular chaperones are also disclosed.

12 Claims, 35 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 24

☐ 22. Document ID: US 6548265 B2

L11: Entry 22 of 53 File: USPT Apr 15, 2003

US-PAT-NO: 6548265
DOCUMENT-IDENTIFIER: US 6548265 B2

TITLE: Treatment or prophylaxis of diseases caused by pilus-forming bacteria

DATE-ISSUED: April 15, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Hultgren; Scott	Ballwin	MO		
Kuehn; Meta	Berkeley	CA		
Xu; Zheng	Blue Bell	PA		
Ogg; Derek	Uppsala			SE
Harris; Mark	Uppsala			SE
Lepisto; Matti	Lund			SE
Jones; Charles Hal	Saint Louis	MO		
Kihlberg; Jan	Dalby			SE

US-CL-CURRENT: 435/7.37; 424/184.1, 424/234.1, 424/241.1, 424/242.1, 435/243, 435/252.8, 435/7.32, 703/11

ABSTRACT:

Novel methods for the treatment and/or prophylaxis of diseases caused by tissue-adhering bacteria are disclosed. By interacting with periplasmic molecular chaperones it is achieved that the assembly of pili is prevented or inhibited and thereby the infectivity of the bacteria is diminished. Also disclosed are methods for screening for drugs as well as methods for the de novo design of such drugs, methods which rely on novel computer drug modelling methods involving an approximative calculation of binding free energy between macromolecules. Finally, novel pyranosides which are believed to be capable of interacting with periplasmic molecular chaperones are also disclosed.

9 Claims, 35 Drawing figures

Exemplary Claim Number: 1
Number of Drawing Sheets: 25

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw. De

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☐ 23. Document ID: US 6451340 B1

L11: Entry 23 of 53 File: USPT Sep 17, 2002

US-PAT-NO: 6451340
DOCUMENT-IDENTIFIER: US 6451340 B1

TITLE: Nucleotide analog compositions

DATE-ISSUED: September 17, 2002

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Arimilli; Murty N.	Fremont	CA		
Kelly; Daphne E.	San Francisco	CA		
Lee; Thomas T. K.	Redwood City	CA		
Manes; Lawrence V.	Moss Beach	CA		
Munger, Jr.; John D.	Alviso	CA		
Prisbe; Ernest J.	Los Altos	CA		
Schultze; Lisa M.	San Carlos	CA		

US-CL-CURRENT: 424/464; 424/465, 424/489, 514/449

ABSTRACT:

The invention provides crystalline forms of adefovir dipivoxil and methods to prepare the crystals. The compositions and methods of the present invention have desirable properties for large scale synthesis of crystalline adefovir dipivoxil or for its formulation into therapeutic dosages. Invention compositions include an anhydrous crystal form of adefovir dipivoxil.

47 Claims, 29 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 29

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw. De

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☐ 24. Document ID: US 6420127 B1

L11: Entry 24 of 53 File: USPT Jul 16, 2002

US-PAT-NO: 6420127
DOCUMENT-IDENTIFIER: US 6420127 B1

TITLE: Compounds and pharmaceutical compositions for the treatment and prophylaxis of bacterial infections

DATE-ISSUED: July 16, 2002

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Hultgren; Scott	Ballwin	MO		
Kuehn; Meta	Berkeley	CA		
Xu; Zheng	Blue Bell	PA		
Ogg; Derek	Uppsala			SE
Harris; Mark	Uppsala			SE
Lepisto; Matti	Lund			SE
Jones; Charles Hal	Saint Louis	MO		
Kihlberg; Jan	Dalby			SE

US-CL-CURRENT: 435/7.37; 424/241.1, 424/242.1, 424/257.1, 435/849

ABSTRACT:

Novel methods for the treatment and/or prophylaxis of diseases caused by tissue-adhering bacteria are disclosed. By interacting with periplasmic molecular chaperones it is achieved that the assembly of pili is prevented or inhibited and thereby the infectivity of the bacteria is diminished. Also disclosed are methods for screening for drugs as well as methods for the de novo design of such drugs, methods which rely on novel computer drug modelling methods involving an approximative calculation of binding free energy between macromolecules. Finally, novel pyranosides which are believed to be capable of interacting with periplasmic molecular chaperones are also disclosed.

9 Claims, 35 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 25

☐ 25. Document ID: US 6403374 B1

L11: Entry 25 of 53 File: USPT Jun 11, 2002

US-PAT-NO: 6403374
DOCUMENT-IDENTIFIER: US 6403374 B1
**** See image for Certificate of Correction ****

TITLE: Long wavelength engineered fluorescent proteins

DATE-ISSUED: June 11, 2002

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Tsien; Roger Y.	La Jolla	CA		

Remington; S. James	Eugene	OR	
Cubitt; Andrew B.	San Diego	CA	
Heim; Roger	Del Mar	CA	
Ormo ; Mats F.	Huddinge		SE

US-CL-CURRENT: 435/325; 435/252.3, 435/252.33, 435/254.11, 435/320.1, 435/410, 536/23.1, 536/23.4, 536/23.6

ABSTRACT:

Engineered fluorescent proteins, nucleic acids encoding them and methods of use are provided.

23 Claims, 55 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 53

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

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☐ 26. Document ID: US 6395745 B1

L11: Entry 26 of 53 File: USPT May 28, 2002

US-PAT-NO: 6395745
DOCUMENT-IDENTIFIER: US 6395745 B1

TITLE: Alkaloid halide salts of swainsonine and methods of use

DATE-ISSUED: May 28, 2002

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Dennis; James W.	Etobicoke			CA
Shah; Rajan N.	Toronto			CA
Ziser; Lothar	Toronto			CA

US-CL-CURRENT: 514/299; 546/183

ABSTRACT:

Crystalline salts of swainsonine, and methods using same.

33 Claims, 13 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 13

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

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☐ 27. Document ID: US 6387890 B1

L11: Entry 27 of 53 File: USPT May 14, 2002

US-PAT-NO: 6387890
DOCUMENT-IDENTIFIER: US 6387890 B1

TITLE: Compositions and methods for inhibiting arginase activity

DATE-ISSUED: May 14, 2002

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Christianson; David	Media	PA		
Baggio; Ricky	Waltham	MA		
Elbaum; Daniel	Newton	MA		

US-CL-CURRENT: 514/64; 562/7

ABSTRACT:

Compositions and methods for inhibiting arginase activity, including arginase activity in a mammal, are provided. Methods of making the compositions of the invention are also provided as are methods of using the compositions therapeutically. The compositions described herein are useful for alleviating or inhibiting a variety of arinase- and NO synthase-related disorders, including heart diseae, gastrointestinal motility disorders, and penile erectile dysfunction in humans.

26 Claims, 47 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 34

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw. De

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☐ 28. Document ID: US 6312887 B1

L11: Entry 28 of 53 File: USPT Nov 6, 2001

US-PAT-NO: 6312887
DOCUMENT-IDENTIFIER: US 6312887 B1
**** See image for Certificate of Correction ****

TITLE: Method of using a crystal of the N-terminal domain of a signal transducer and activator of transcription

DATE-ISSUED: November 6, 2001

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Vinkemeier; Uwe	New York	NY		
Moarefi; Ismail	Martinsried			DE

Darnell, Jr.; James E.	Larchmont	NY
Kuriyan; John	Riverdale	NY

US-CL-CURRENT: 435/4; 435/6, 436/86, 702/19

ABSTRACT:

The present invention provides a crystal containing the N-terminal domain of a STAT protein that is of sufficient quality to perform X-ray crystallographic studies. Methods of preparing the crystals are include in the invention. The present invention further discloses the three-dimensional structure of the crystal. The present invention also provides methods of using the structural information in drug discovery and drug development.

16 Claims, 9 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 6

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw De

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☐ 29. Document ID: US 6266622 B1

L11: Entry 29 of 53 File: USPT Jul 24, 2001

US-PAT-NO: 6266622
DOCUMENT-IDENTIFIER: US 6266622 B1

TITLE: Nuclear receptor ligands and ligand binding domains

DATE-ISSUED: July 24, 2001

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Scanlan; Thomas S.	San Francisco	CA		
Baxter; John D.	San Francisco	CA		
Fletterick; Robert J.	San Francisco	CA		
Wagner; Richard L.	San Francisco	CA		
Kushner; Peter J.	San Francisco	CA		
Apriletti; James J.	Berkeley	CA		
West; Brian L.	San Francisco	CA		
Shiau; Andrew K.	San Francisco	CA		

US-CL-CURRENT: 702/22; 530/350, 702/19, 702/20

ABSTRACT:

The present invention provides new methods, particularly computational methods, and compositions for the generation of nuclear receptor synthetic ligands based on the three dimensional structure of nuclear receptors, particularly the thyroid receptor (herein referred to as "TR"). Also provided are crystals, nuclear receptor synthetic ligands, and related methods.

28 Claims, 52 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 50

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw D

☐ 30. Document ID: US 6251620 B1

L11: Entry 30 of 53 File: USPT Jun 26, 2001

US-PAT-NO: 6251620
DOCUMENT-IDENTIFIER: US 6251620 B1

TITLE: Three dimensional structure of a ZAP tyrosine protein kinase fragment and modeling methods

DATE-ISSUED: June 26, 2001

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Hatada; Marcos H.	Charlestown	MA		
Lu; Xiaode	Revere	MA		
Laird; Ellen R.	Newton	MA		
Karas; Jennifer L.	Lexington	MA		
Zoller; Mark J.	Weston	MA		
Holt; Dennis A.	Stow	MA		

US-CL-CURRENT: 435/15; 435/194, 436/86, 530/350, 702/19

ABSTRACT:

The invention relates to human ZAP-70, and in particular, to the region of ZAP-70 containing the tandem Src homology-2 ("SH2") domains, to crystalline forms thereof, liganded or unliganded, which are particularly useful for the determination of the three-dimensional structure of the protein. The three dimensional structure of the tandem SH2 region of ZAP provides information useful for the design of pharmaceutical compositions which inhibit the biological function of ZAP and other members of the ZAP family of SH2 domain-containing proteins, particularly those biological functions mediated by molecular interactions involving one or both SH2 domains.

7 Claims, 15 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 14

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw D

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Hit List

First Hit | Clear | Generate Collection | Print | Fwd Refs | Bkwd Refs | Generate OACS

Search Results - Record(s) 31 through 53 of 53 returned.

☐ 31. Document ID: US 6236946 B1

Using default format because multiple data bases are involved.

L11: Entry 31 of 53 File: USPT May 22, 2001

US-PAT-NO: 6236946
DOCUMENT-IDENTIFIER: US 6236946 B1

TITLE: Nuclear receptor ligands and ligand binding domains

DATE-ISSUED: May 22, 2001

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Scanlan; Thomas S.	San Francisco	CA	94122	
Baxter; John D.	San Francisco	CA	94127	
Fletterick; Robert J.	San Francisco	CA	94131	
Wagner; Richard L.	San Francisco	CA	94117	
Kushner; Peter J.	San Francisco	CA	94122	
Apriletti; James	Berkeley	CA	94702	
West; Brian	San Francisco	CA	94110	
Shiau; Andrew K.	San Francisco	CA	94122	

US-CL-CURRENT: 702/22; 530/350, 702/19, 702/20

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw D

☐ 32. Document ID: US 6156526 A

L11: Entry 32 of 53 File: USPT Dec 5, 2000

US-PAT-NO: 6156526
DOCUMENT-IDENTIFIER: US 6156526 A
**** See image for Certificate of Correction ****

TITLE: Crystal of a Ras-Sos complex and methods of use thereof

DATE-ISSUED: December 5, 2000

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Boriack-Sjodin; Ann	Watertown	MA		

Margarit; S. Mariana	Setauket	NY
Bar-Sagi; Dafna	Stony Brook	NY
Cole; Philip	New York	NY
Kuriyan; John	Riverdale	NY

US-CL-CURRENT: 435/18; 435/195, 530/350, 702/19, 702/22

ABSTRACT:

A detailed three-dimensional structure for the complex formed between Ras and the Son of sevenless (Sos) protein is provided. Crystals of this complex are also included in the invention. The present invention farther provides procedures for identifying agents that can inhibit tumor proliferation through the use of rational drug design predicated on the crystals and crystallographic data disclosed.

32 Claims, 104 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 97

☐ 33. Document ID: US 6153396 A

L11: Entry 33 of 53 File: USPT Nov 28, 2000

US-PAT-NO: 6153396
DOCUMENT-IDENTIFIER: US 6153396 A

TITLE: Treatment or prophylaxis of diseases caused by pilus-forming bacteria

DATE-ISSUED: November 28, 2000

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Hultgren; Scott	Ballwin	MO		
Kuehn; Meta	Berkeley	CA		
Xu; Zheng	Blue Bell	PA		
Ogg; Derek	Uppsala			SE
Harris; Mark	Uppsala			SE
Lepisto ; Matti	Lund			SE
Kihlberg; Jan	Dalby			SE
Jones; Charles Hal	St. Louis	MO		

US-CL-CURRENT: 435/7.32; 424/241.1, 424/242.1, 424/257.1, 435/7.37, 435/849

ABSTRACT:

Novel methods for the treatment and/or prophylaxis of diseases caused by tissue-adhering bacteria are disclosed. By interacting with periplasmic molecular chaperones it is achieved that the assembly of pili is prevented or inhibited and thereby the infectivity of the bacteria is diminished. Also disclosed are methods

for screening for drugs as well as methods for the de novo design of such drugs, methods which rely on novel computer drug modelling methods involving an approximative calculation of binding free energy between macromolecules. Finally, novel pyranosides which are believed to be capable of interacting with periplasmic molecular chaperones are also disclosed.

10 Claims, 29 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 24

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Drawi De

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☐ 34. Document ID: US 6117663 A

L11: Entry 34 of 53 File: USPT Sep 12, 2000

US-PAT-NO: 6117663
DOCUMENT-IDENTIFIER: US 6117663 A
**** See image for Certificate of Correction ****

TITLE: Crystal of a Ras-Sos complex

DATE-ISSUED: September 12, 2000

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Boriack-Sjodin; Ann	Waltham	MA		
Margarit; S. Mariana	Setauket	NY		
Bar-Sagi; Dafna	Stony Brook	NY		
Cole; Philip	Baltimore	MD		
Kuriyan; John	Riverdale	NY		

US-CL-CURRENT: 435/195; 435/18, 530/350

ABSTRACT:

A detailed three-dimensional structure for the complex formed between Ras and the Son of sevenless (Sos) protein is provided. Crystals of this complex are also included in the invention. The present invention further provides procedures for identifying agents that can inhibit tumor proliferation through the use of rational drug design predicated on the crystals and crystallographic data disclosed.

10 Claims, 22 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 16

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Drawi De

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☐ 35. Document ID: US 6110672 A

L11: Entry 35 of 53 File: USPT Aug 29, 2000

US-PAT-NO: 6110672
DOCUMENT-IDENTIFIER: US 6110672 A

TITLE: Peripheral nervous system specific sodium channels, DNA encoding therefor, crystallization, X-ray diffraction, computer molecular modeling, rational drug design, drug screening, and methods of making and using thereof

DATE-ISSUED: August 29, 2000

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Mandel; Gail	Stony Brook	NY		
Halegoua; Simon	Belle Terre	NY		

US-CL-CURRENT: 435/6; 435/320.1, 435/325, 435/455, 435/91.41, 536/23.1, 536/23.2, 536/23.5, 536/24.3, 536/24.31

ABSTRACT:

Cloning, expression, viral and delivery vectors and hosts which contain nucleic acid coding for at least one peripheral nervous system specific (PNS) sodium channel peptide (SCP), isolated PNS SCP, and compounds and compositions and methods, are provided, for isolating, crystallizing, x-ray analysing molecular modeling, rational drug designing, selecting, making and using therapeutic or diagnostic agents or ligands having at least one peripheral nervous system specific (PNS) sodium channel (SC) modulating activity.

15 Claims, 14 Drawing figures
Exemplary Claim Number: 13
Number of Drawing Sheets: 35

☐ 36. Document ID: US 6093573 A

L11: Entry 36 of 53 File: USPT Jul 25, 2000

US-PAT-NO: 6093573
DOCUMENT-IDENTIFIER: US 6093573 A

TITLE: Three-dimensional structure of bactericidal/permeability-increasing protein (BPI)

DATE-ISSUED: July 25, 2000

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Beamer; Lesa J.	Santa Monica	CA		
Carroll; Stephen F.	Walnut Creek	CA		
Eisenberg; David	Los Angeles	CA		

US-CL-CURRENT: 436/86; 530/350, 702/19, 702/22

ABSTRACT:

The present invention provides a crystallized Bactericidal Permeability-Increasing (BPI) protein; methods for x-ray diffraction analysis to provide x-ray diffraction patterns of sufficiently high resolution for three-dimensional structure determination of the protein, as well as methods for rational drug design, based on using amino acid sequence data and/or x-ray crystallography data provided on computer readable media, as analyzed on a computer system having suitable computer algorithms; and atomic coordinates are provided yielding structural information on the lipid binding and lipid transport protein family that includes BPI, LBP, CETP and PLTP.

6 Claims, 126 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 125

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw De

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☐ 37. Document ID: US 6087478 A

L11: Entry 37 of 53 File: USPT Jul 11, 2000

US-PAT-NO: 6087478
DOCUMENT-IDENTIFIER: US 6087478 A
**** See image for Certificate of Correction ****

TITLE: Crystal of the N-terminal domain of a STAT protein and methods of use thereof

DATE-ISSUED: July 11, 2000

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Vinkemeier; Uwe	New York	NY		
Moarefi; Ismail	Martinsried			DE
Darnell, Jr.; James E.	Larchmont	NY		
Kuriyan; John	Riverdale	NY		

US-CL-CURRENT: 530/350; 435/69.1, 436/86, 530/421, 702/19

ABSTRACT:

The present invention provides a crystal containing the N-terminal domain of a STAT protein that is of sufficient quality to perform X-ray crystallographic studies. Methods of preparing the crystals are include in the invention. The present invention further discloses the three-dimensional structure of the crystal. The present invention also provides methods of using the structural information in drug discovery and drug development.

5 Claims, 9 Drawing figures
Exemplary Claim Number: 1

Number of Drawing Sheets: 6

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw. De

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☐ 38. Document ID: US 6077824 A

L11: Entry 38 of 53 File: USPT Jun 20, 2000

US-PAT-NO: 6077824
DOCUMENT-IDENTIFIER: US 6077824 A
**** See image for Certificate of Correction ****

TITLE: Methods for improving the activity of .delta.-endotoxins against insect pests

DATE-ISSUED: June 20, 2000

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
English; Leigh H.	Churchville	PA		
Brussock; Susan M.	New Hope	PA		
Malvar; Thomas M.	St. Louis	MO		
Bryson; James W.	Langhorne	PA		
Kulesza; Caroline A.	Charlottesville	VA		
Walters; Frederick S.	Beaver Falls	PA		
Slatin; Stephen L.	Fair Lawn	NJ		
Von Tersch; Michael A.	Erving Township	NJ		

US-CL-CURRENT: 514/12; 435/69.1, 514/2, 530/350, 530/402

ABSTRACT:

Disclosed are methods for increasing the activity of B. thuringiensis .delta.-endotoxins against Coleopteran insect pests. Also disclosed are methods for mutagenizing nucleic acid sequences encoding these polypeptides, and increasing insect resistance in transgenic plants expressing these genes.

41 Claims, 23 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw. De

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☐ 39. Document ID: US 6077707 A

L11: Entry 39 of 53 File: USPT Jun 20, 2000

US-PAT-NO: 6077707
DOCUMENT-IDENTIFIER: US 6077707 A

TITLE: Long wavelength engineered fluorescent proteins

DATE-ISSUED: June 20, 2000

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Tsien; Roger Y.	La Jolla	CA		
Remington; S. James	Eugene	OR		
Cubitt; Andrew B.	San Diego	CA		
Heim; Roger	Del Mar	CA		
Ormo; Mats F.	Huddinge			SE

US-CL-CURRENT: 435/325; 435/252.3, 435/252.33, 435/254.11, 435/320.1, 435/410, 435/69.1, 530/350, 536/23.1, 536/23.5

ABSTRACT:

This invention provides functional engineered fluorescent proteins with varied fluorescence characteristics that can be easily distinguished from currently existing green and blue fluorescent proteins. In one aspect, the invention provides nucleic acids, expression vectors and recombinant host cells comprising nucleotide sequences encoding functional engineered fluorescent proteins comprising aromatic substitutions at position 66 and a folding mutation. In one embodiment the invention provides for fluorescent proteins containing an aromatic substitution at Thr 203.

17 Claims, 53 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 53

☐ 40. Document ID: US 6057091 A

L11: Entry 40 of 53 File: USPT May 2, 2000

US-PAT-NO: 6057091
DOCUMENT-IDENTIFIER: US 6057091 A

TITLE: Method of identifying compounds affecting hedgehog cholesterol transfer

DATE-ISSUED: May 2, 2000

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Beachy; Philip A.	Baltimore	MD		
Porter; Jeffrey A.	Belmont	MA		

US-CL-CURRENT: 435/4; 436/71, 530/300, 530/350

ABSTRACT:

The present invention provides two novel polypeptides, referred to as the "N" and "C" fragments of hedgehog, or N-terminal and C-terminal fragments, respectively, which are derived after specific cleavage at a G.sup..dwnarw. CF site recognized by the autoproteolytic domain in the native protein. Also included are sterol-modified hedgehog polypeptides and functional fragments thereof. Methods of identifying compositions which affect hedgehog activity based on inhibition of cholesterol modification of hedgehog protein are described.

4 Claims, 126 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 54

☐ 41. Document ID: US 6054321 A

L11: Entry 41 of 53 File: USPT Apr 25, 2000

US-PAT-NO: 6054321
DOCUMENT-IDENTIFIER: US 6054321 A

TITLE: Long wavelength engineered fluorescent proteins

DATE-ISSUED: April 25, 2000

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Tsien; Roger Y.	La Jolla	CA		
Remington; S. James	Eugene	OR		
Cubitt; Andrew B.	San Diego	CA		
Heim; Roger	Del Mar	CA		
Ormo; Mats F.	Huddinge			SE

US-CL-CURRENT: 436/86; 530/350, 702/19, 702/22

ABSTRACT:

This invention provides functional engineered fluorescent proteins with varied fluorescence characteristics that can be easily distinguished from currently existing green and blue fluorescent proteins. In one embodiment the invention provides for the three dimensional structure and atomic coordinates of an Aequorea green fluorescent protein and methods for their use. In one embodiment, this invention provides a computational method of modeling the three dimensional structure of any other fluorescent protein based on the three dimensional structure of an Aequorea green fluorescent protein.

15 Claims, 36 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 53

☐ 42. Document ID: US 6020162 A

L11: Entry 42 of 53 File: USPT Feb 1, 2000

US-PAT-NO: 6020162
DOCUMENT-IDENTIFIER: US 6020162 A

TITLE: Crystal of a protein-ligand complex containing an N-terminal truncated eIF4E, and methods of use thereof

DATE-ISSUED: February 1, 2000

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Burley; Stephen K.	New York	NY		
Sonenberg; Nahum	Cote St-Luc			CA
Marcotrigiano; Joseph	New York	NY		
Gingras; Anne-Claude	Montreal			CA

US-CL-CURRENT: 435/69.1; 435/252.3, 435/320.1, 536/23.5

ABSTRACT:

A detailed three-dimensional structure for the least abundant of the general translation initiation factors in eukaryotes, eIF4E, complexed with a ligand is disclosed. The novel N-terminal truncated eIF4Es which were constructed so as to omit a significant portion of the flexible N-terminal tail of the eIF4E are also part of the present invention. In addition, the crystals of the protein-ligand complexes containing the N-terminal truncated eIF4Es are also included. Furthermore, methods of identifying antagonists of the eIF4E protein which can be used to regulate protein synthesis in cells are also disclosed.

6 Claims, 13 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 6

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw De

☐ 43. Document ID: US 6001823 A

L11: Entry 43 of 53 File: USPT Dec 14, 1999

US-PAT-NO: 6001823
DOCUMENT-IDENTIFIER: US 6001823 A

TITLE: Treatment or prophylaxis of diseases caused by pilus-forming bacteria

DATE-ISSUED: December 14, 1999

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Hultgren; Scott	Ballwin	MO		
Kuehn; Meta	Berkeley	CA	94705	
Xu; Zheng	Blue Bell	PA	19422	
Ogg; Derek	Uppsala			SE
Harris; Mark	S-756 45 Uppsala			SE
Lepisto ; Matti	S-224 73 Lund			SE
Kihlberg; Jan	S-240 10 Dalby			SE
Jones; Charles Hal	St. Louis	MO	63110	

US-CL-CURRENT: 514/99; 514/382, 514/459, 514/460, 548/252, 548/253, 549/216, 549/416, 549/417, 549/419, 549/420

ABSTRACT:

Novel methods for the treatment and/or prophylaxis of diseases caused by tissue-adhering bacteria are disclosed. By interacting with periplasmic molecular chaperones it is achieved that the assembly of pili is prevented or inhibited and thereby the infectivity of the bacteria is diminished. Also disclosed are methods for screening for drugs as well as methods for the de novo design of such drugs, methods which rely on novel computer drug modelling methods involving an approximative calculation of binding free energy between macromolecules. Finally, novel pyranosides which are believed to be capable of interacting with periplasmic molecular chaperones are also disclosed.

5 Claims, 34 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 24

☐ 44. Document ID: US 5939528 A

L11: Entry 44 of 53 File: USPT Aug 17, 1999

US-PAT-NO: 5939528
DOCUMENT-IDENTIFIER: US 5939528 A

TITLE: Crystalline FRAP complex

DATE-ISSUED: August 17, 1999

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Clardy; Jon C.	Ithaca	NY		
Choi; Jungwon	Seoul			KR

US-CL-CURRENT: 530/350; 536/23.1, 536/23.5

ABSTRACT:

The invention relates to the human protein FRAP, and in particular to the FKBP12-rapamycin binding domain thereof and to the ternary complex formed by the FRB domain, rapamycin and FKBP12. A new crystalline composition comprising the ternary complex, coordinates defining its three dimensional structure in atomic detail, and uses thereof are disclosed.

3 Claims, 39 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 39

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw. D

☐ 45. Document ID: US 5872011 A

L11: Entry 45 of 53 File: USPT Feb 16, 1999

US-PAT-NO: 5872011
DOCUMENT-IDENTIFIER: US 5872011 A

TITLE: Crystal of a protein-ligand complex containing an N-terminal truncated eIF4E, and methods of use thereof

DATE-ISSUED: February 16, 1999

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Burley; Stephen K.	New York	NY		
Sonenberg; Nahum	Cote St-Luc			CA
Marcotrigiano; Joseph	New York	NY		
Gingras; Anne-Claude	Montreal			CA

US-CL-CURRENT: 436/501; 530/350

ABSTRACT:

A detailed three-dimensional structure for the least abundant of the general translation initiation factors in eukaryotes, eIF4E, complexed with a ligand is disclosed. The novel N-terminal truncated eIF4Es which were constructed so as to omit a significant portion of the flexible N-terminal tail of the eIF4E are also part of the present invention. In addition, the crystals of the protein-ligand complexes containing the N-terminal truncated eIF4Es are also included. Furthermore, methods of identifying antagonists of the eIF4E protein which can be used to regulate protein synthesis in cells are also disclosed.

21 Claims, 15 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 6

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw. D

☐ 46. Document ID: US 5814575 A

L11: Entry 46 of 53 File: USPT Sep 29, 1998

US-PAT-NO: 5814575
DOCUMENT-IDENTIFIER: US 5814575 A

TITLE: Chromium compounds and uses thereof

DATE-ISSUED: September 29, 1998

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Reagen; William K.	Stillwater	MN		
Pettijohn; Ted M.	Bartlesville	OK		
Freeman; Jeffrey W.	Bartlesville	OK		

US-CL-CURRENT: 502/117; 502/104, 502/108, 502/120, 526/141, 585/513

ABSTRACT:

Novel chromium-containing compounds, such as, for example, chromium pyrrolides, are prepared by forming a mixture of a chromium salt, a metal amide, and an electron pair donor solvent, such as, for example, an ether. These novel chromium-containing, or chromium pyrrolide, compounds can be used either unsupported or supported on an inorganic oxide support, with a metal alkyl and an unsaturated hydrocarbon, to trimerize, oligomerize, and/or polymerize olefins.

27 Claims, 9 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 9

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Drawi De

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☐ 47. Document ID: US 5786431 A

L11: Entry 47 of 53 File: USPT Jul 28, 1998

US-PAT-NO: 5786431
DOCUMENT-IDENTIFIER: US 5786431 A

TITLE: Process for olefin polymerization

DATE-ISSUED: July 28, 1998

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Reagen; William K.	Stillwater	MN		
Pettijohn; Ted M.	Marshall	TX		
Freeman; Jeffrey W.	Bartlesville	OK		
Benham; Elizabeth A.	Bartlesville	OK		

US-CL-CURRENT: 526/113; 526/114, 526/118, 526/119, 526/96, 526/97

ABSTRACT:

Novel chromium-containing compounds are prepared by forming a mixture of a chromium salt, a metal amide, and an ether. These novel chromium-containing, or chromium pyrrolide, compounds, with a metal alkyl and an unsaturated hydrocarbon, can be used as a cocatalyst system in the presence of an olefin polymerization catalyst system to produce a comonomer in-situ. The resultant polymer, although produced from predominately one monomer, has characteristics of a copolymer.

30 Claims, 9 Drawing figures
Exemplary Claim Number: 1,3
Number of Drawing Sheets: 9

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

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☐ 48. Document ID: US 5763723 A

L11: Entry 48 of 53 File: USPT Jun 9, 1998

US-PAT-NO: 5763723
DOCUMENT-IDENTIFIER: US 5763723 A

TITLE: Chromium compounds and uses thereof

DATE-ISSUED: June 9, 1998

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Reagen; William K.	Stillwater	MN		
Pettijohn; Ted M.	Bartlesville	OK		
Freeman; Jeffrey W.	Bartlesville	OK		

US-CL-CURRENT: 585/513; 585/511

ABSTRACT:

Novel chromium-containing compounds, such as, for example, chromium pyrrolides, are prepared by forming a mixture of a chromium salt, a metal amide, and an electron pair donor solvent, such as, for example, an ether. These novel chromium-containing, or chromium pyrrolide, compounds can be used either unsupported or supported on an inorganic oxide support, with a metal alkyl and an unsaturated hydrocarbon, to trimerize, oligomerize, and/or polymerize olefins.

6 Claims, 9 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 9

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

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☐ 49. Document ID: US 5523507 A

L11: Entry 49 of 53 File: USPT Jun 4, 1996

US-PAT-NO: 5523507
DOCUMENT-IDENTIFIER: US 5523507 A
**** See image for Certificate of Correction ****

TITLE: Process of trimerizing and oligomerizing olefins using chromium compounds

DATE-ISSUED: June 4, 1996

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Reagen; William K.	Stillwater	MN		
Pettijohn; Ted M.	Bartlesville	OK		
Freeman; Jeffrey W.	Bartlesville	OK		

US-CL-CURRENT: 585/513; 585/511, 585/512, 585/522, 585/523

ABSTRACT:

Novel chromium-containing compounds, such as, for example, chromium pyrrolides, are prepared by forming a mixture of a chromium salt, a metal amide, and an electron pair donor solvent, such as, for example, an ether. These novel chromium-containing, or chromium pyrrolide, compounds can be used either unsupported or supported on an inorganic oxide support, with a metal alkyl and an unsaturated hydrocarbon, to trimerize, oligomerize, and/or polymerize olefins.

28 Claims, 9 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 9

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Drawi De

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☐ 50. Document ID: US 5451645 A

L11: Entry 50 of 53 File: USPT Sep 19, 1995

US-PAT-NO: 5451645
DOCUMENT-IDENTIFIER: US 5451645 A

TITLE: Process for olefin polymerization

DATE-ISSUED: September 19, 1995

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Reagen; William K.	Idaho Falls	ID		
Pettijohn; Ted M.	Bartlesville	OK		
Freeman; Jeffrey W.	Bartlesville	OK		

Benham; Elizabeth A. Bartlesville OK

US-CL-CURRENT: 526/97; 526/114, 526/115, 526/119, 526/121, 526/127, 526/133, 526/137, 526/141

ABSTRACT:

Novel chromium-containing compounds are prepared by forming a mixture of a chromium salt, a metal amide, and an ether. These novel chromium-containing, or chromium pyrrolide, compounds, with a metal alkyl and an unsaturated hydrocarbon, can be used as a cocatalyst system in the presence of an olefin polymerization catalyst system to produce a comonomer in-situ. The resultant polymer, although produced from predominately one monomer, has characteristics of a copolymer.

29 Claims, 9 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 9

☐ 51. Document ID: US 5376612 A

L11: Entry 51 of 53 File: USPT Dec 27, 1994

US-PAT-NO: 5376612
DOCUMENT-IDENTIFIER: US 5376612 A
**** See image for Certificate of Correction ****

TITLE: Chromium catalysts and process for making chromium catalysts

DATE-ISSUED: December 27, 1994

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Reagen; William K.	Idaho Falls	ID		
Pettijohn; Ted M.	Bartlesville	OK		
Freeman; Jeffrey W.	Bartlesville	OK		

US-CL-CURRENT: 502/104; 502/107, 502/108, 502/110, 502/112, 502/113, 502/117, 502/119, 502/120, 502/123, 502/124, 502/130, 502/131, 502/167, 526/110, 526/111, 526/114, 526/124.1, 526/127, 526/133, 526/136, 526/137, 526/141, 526/97

ABSTRACT:

Novel chromium-containing compounds, such as, for example, chromium pyrrolides, are prepared by forming a mixture of a chromium salt, a metal amide, and an electron pair donor solvent, such as, for example, an ether. These novel chromium-containing, or chromium pyrrolide, compounds can be used either unsupported or supported on an inorganic oxide support, with a metal alkyl and an unsaturated hydrocarbon, to trimerize, oligomerize, and/or polymerize olefins.

30 Claims, 9 Drawing figures
Exemplary Claim Number: 1

Number of Drawing Sheets: 9

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

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☐ 52. Document ID: US 4980462 A

L11: Entry 52 of 53 File: USPT Dec 25, 1990

US-PAT-NO: 4980462
DOCUMENT-IDENTIFIER: US 4980462 A

TITLE: Antiviral agents

DATE-ISSUED: December 25, 1990

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Karlsson; Karl-Anders	Gothenburg			SE
Norrby; Erling	Lidingo			SE
Wadell; Goran	Ume.ang.			SE

US-CL-CURRENT: 536/53; 424/520, 514/25, 514/53, 514/613, 514/625, 536/115, 536/116, 536/118, 536/120, 536/122, 536/4.1, 536/54, 536/55

ABSTRACT:

A second-step virus binding receptor is found in nature on the surface of animal and plant cells. This receptor is thought to be needed for virus penetration into target cells. The second-step receptor has been found to bind a wide variety of viruses belonging to a number of different families. The second-step receptor and natural or synthetic substances which correspond to or are analogous to the binding epitope of the second-step receptor in that they are able to bind to a site on the virus which recognizes the binding epitope of the natural second-step receptor, are therefore indicated for the diagnosis, prophylaxis or treatment of viral infections.

15 Claims, 9 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 9

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

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☐ 53. Document ID: US 4859769 A

L11: Entry 53 of 53 File: USPT Aug 22, 1989

US-PAT-NO: 4859769
DOCUMENT-IDENTIFIER: US 4859769 A

TITLE: Antiviral agents

DATE-ISSUED: August 22, 1989

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Karlsson; Karl-Anders	Gothenburg			SE
Norrby; Erling	Lidingo			SE
Wadell; Goran	Ume.ang.			SE

US-CL-CURRENT: 514/25; 514/53, 514/613, 514/625, 536/115, 536/116, 536/118, 536/120, 536/122, 536/123.13, 536/4.1, 536/54, 536/55

ABSTRACT:

A second-step virus binding receptor is found in nature on the surface of animal and plant cells. This receptor is thought to be needed for virus penetration into target cells. The second-step receptor has been found to bind a wide variety of viruses belonging to a number of different families. The second-step receptor and natural or synthetic substances which correspond to or are analogous to the binding epitope of the second-step receptor in that they are able to bind to a site on the virus which recognizes the binding epitope of the natural second-step receptor, are therefore indicated for the diagnosis, prophylaxis or treatment of viral infections.

13 Claims, 9 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 9

Terms	Documents
L5 and reflection	53

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☐ 1. Document ID: US 20060004067 A1

L9: Entry 1 of 101 File: PGPB Jan 5, 2006

PGPUB-DOCUMENT-NUMBER: 20060004067
PGPUB-FILING-TYPE:
DOCUMENT-IDENTIFIER: US 20060004067 A1

TITLE: Process for preparing 2-aminothiazole-5-aromatic carboxamides as kinase inhibitors

PUBLICATION-DATE: January 5, 2006

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Chen; Bang-Chi	Plainsboro	NJ	US
Droghini; Roberto	Candiac	NJ	CA
Lajeunesse; Jean	Candiac	NJ	CA
DiMarco; John D.	East Brunswick	NJ	US
Galella; Michael	Kendall Park		US
Chidambaram; Ramakrishnan	Pennington		US

US-CL-CURRENT: 514/370; 548/181, 548/195

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

☐ 2. Document ID: US 20060003931 A1

L9: Entry 2 of 101 File: PGPB Jan 5, 2006

PGPUB-DOCUMENT-NUMBER: 20060003931
PGPUB-FILING-TYPE:
DOCUMENT-IDENTIFIER: US 20060003931 A1

TITLE: Crystal structure of the hepatocyte growth factor and methods of use

PUBLICATION-DATE: January 5, 2006

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Eigenbrot; Charles W. JR.	Burlingame	CA	US
Kirchhofer; Daniel K.	Los Altos	CA	US

Lazarus; Robert A. Millbrae CA US

US-CL-CURRENT: 514/12; 530/399, 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw D

☐ 3. Document ID: US 20060003432 A1

L9: Entry 3 of 101 File: PGPB Jan 5, 2006

PGPUB-DOCUMENT-NUMBER: 20060003432
PGPUB-FILING-TYPE:
DOCUMENT-IDENTIFIER: US 20060003432 A1

TITLE: Novel purified polypeptides from enterococcus faecalis

PUBLICATION-DATE: January 5, 2006

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Edwards; Aled	Toronto		CA
Dharamsi; Akil	Richmond Hill		CA
Vedadi; Masoud	Toronto		CA
Beattie; Bryan	Oakville		CA
Clarke; Teresa	Toronto		CA
Kimber; Matthew	Toronto		CA

US-CL-CURRENT: 435/199; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw D

☐ 4. Document ID: US 20050288279 A1

L9: Entry 4 of 101 File: PGPB Dec 29, 2005

PGPUB-DOCUMENT-NUMBER: 20050288279
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050288279 A1

TITLE: Phenothiazine derivatives and their method of use

PUBLICATION-DATE: December 29, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Rozman, Karl K.	Shawnee Mission	KS	US
Fried, Kristian	Idstein	KS	DE
Terranova, Paul F.	Overland Park	KS	US
Georg, Gunda I.	Lawrence	KS	US

Dutta, Apurba Lawrence US

US-CL-CURRENT: 514/224.8; 544/39

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

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☐ 5. Document ID: US 20050272681 A1

L9: Entry 5 of 101 File: PGPB Dec 8, 2005

PGPUB-DOCUMENT-NUMBER: 20050272681
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050272681 A1

TITLE: Ribosome structure and protein synthesis inhibitors

PUBLICATION-DATE: December 8, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Steitz, Thomas A.	Branford	CT	US
Moore, Peter B.	North Haven	CT	US
Sutcliffe, Joyce A.	Clinton	CT	US
Oyelere, Adegboyega K.	New Haven	CT	US
Ippolito, Joseph A.	Guilford	CT	US

US-CL-CURRENT: 514/44; 536/23.1

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

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☐ 6. Document ID: US 20050266515 A1

L9: Entry 6 of 101 File: PGPB Dec 1, 2005

PGPUB-DOCUMENT-NUMBER: 20050266515
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050266515 A1

TITLE: Glyceraldehyde 3-phosphate dehydrogenase-S (GAPDHS), a glycolytic anzyme expressed only in male germ cells, is a target for male contraception

PUBLICATION-DATE: December 1, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
O'Brien, Deborah A.	Chapell Hill	NC	US
Eddy, Edward M.	Chapel Hill	NC	US

US-CL-CURRENT: 435/25; 514/169, 514/2, 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw D

☐ 7. Document ID: US 20050261183 A1

L9: Entry 7 of 101 File: PGPB Nov 24, 2005

PGPUB-DOCUMENT-NUMBER: 20050261183
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050261183 A1

TITLE: PTHrP-derived modulators of smooth muscle proliferation

PUBLICATION-DATE: November 24, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Stewart, Andrew F.	Pittsburgh	PA	US
Fiaschi-Taesch, Nathalie	Pittsburgh	PA	US

US-CL-CURRENT: 514/12; 435/235.1, 435/320.1, 435/325, 435/69.4, 530/388.24, 530/399

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw D

☐ 8. Document ID: US 20050250195 A1

L9: Entry 8 of 101 File: PGPB Nov 10, 2005

PGPUB-DOCUMENT-NUMBER: 20050250195
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050250195 A1

TITLE: Crystallographic structure of TcPRACA and uses therefor

PUBLICATION-DATE: November 10, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Minoprio, Paola	Villiers sur Marne		FR
Alzari, Pedro	Paris		FR
Buschiazzo, Alejandro	Paris		FR
Gregoire, Christophe	Parede PaVegol		FR
Berneman, Armand	Paris		FR
Degrave, Wim M.	Rio De Janieiro		BR

US-CL-CURRENT: 435/232; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw D

☐ 9. Document ID: US 20050245728 A1

L9: Entry 9 of 101 File: PGPB Nov 3, 2005

PGPUB-DOCUMENT-NUMBER: 20050245728
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050245728 A1

TITLE: Novel purified polypeptides from Pseudomonas aeruginosa

PUBLICATION-DATE: November 3, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Edwards, Aled	Toronto		CA
Dharamsi, Akil	Richmond Hill		CA
Vedadi, Masoud	Toronto		CA
Kimber, Matthew	Toronto		CA
Vallee, Francois	Toronto		CA

US-CL-CURRENT: 530/350; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw De

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☐ 10. Document ID: US 20050244939 A1

L9: Entry 10 of 101 File: PGPB Nov 3, 2005

PGPUB-DOCUMENT-NUMBER: 20050244939
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050244939 A1

TITLE: Variant aldolase and processes for producing an optically active IHOG and an optically active monatin using the same

PUBLICATION-DATE: November 3, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Sugiyama, Masakazu	Kawasaki-shi		JP
Kashiwagi, Tatsuki	Kawasaki-shi		JP
Mori, Kenichi	Kawasaki-shi		JP
Suzuki, Eiichiro	Kawasaki-shi		JP

US-CL-CURRENT: 435/121; 435/193, 435/252.34, 435/471, 435/69.1, 536/23.2

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw De

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☐ 11. Document ID: US 20050239186 A1

L9: Entry 11 of 101 File: PGPB Oct 27, 2005

PGPUB-DOCUMENT-NUMBER: 20050239186
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050239186 A1

TITLE: Peptidyl-tRNA hydrolase of Enterococcus faecalis

PUBLICATION-DATE: October 27, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Edwards, Aled	Toronto		CA
Dharamsi, Akil	Richmond Hill		CA
Vedadi, Masoud	Toronto		CA
Beattie, Bryan	Oakville		CA
Kimber, Matthew	Toronto		CA

US-CL-CURRENT: 435/199; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

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☐ 12. Document ID: US 20050234227 A1

L9: Entry 12 of 101 File: PGPB Oct 20, 2005

PGPUB-DOCUMENT-NUMBER: 20050234227
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050234227 A1

TITLE: Ribosome structure and protein synthesis inhibitors

PUBLICATION-DATE: October 20, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Steitz, Thomas A.	Branford	CT	US
Moore, Peter B.	North Haven	CT	US
Ban, Nenad	Zurich	SC	CH
Nissen, Poul	Aarhus N		DK
Hansen, Jeffrey	Charleston		US

US-CL-CURRENT: 536/23.1; 435/199, 702/20

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

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☐ 13. Document ID: US 20050233349 A1

L9: Entry 13 of 101 File: PGPB Oct 20, 2005

PGPUB-DOCUMENT-NUMBER: 20050233349
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050233349 A1

TITLE: Crystal structure of ribosomal protein L11/GTPase activating region rRNA and uses thereof

PUBLICATION-DATE: October 20, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Wimberly, Brian T.	Guilford	CT	US
Ramakrishnan, Venkatraman	Cambridge		GB

US-CL-CURRENT: 435/6; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

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☐ 14. Document ID: US 20050221462 A1

L9: Entry 14 of 101 File: PGPB Oct 6, 2005

PGPUB-DOCUMENT-NUMBER: 20050221462
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050221462 A1

TITLE: Novel purified polypeptides from pseudomonas aeruginosa

PUBLICATION-DATE: October 6, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Edwards, Aled	Toronto		CA
Dharamsi, Akil	Richmond Hill		CA
Vedadi, Masoud	Toronto		CA
Domagala, Megan	Woodstock		CA
Kimber, Matthew	Toronto		CA
Vallee, Francois	Toronto		CA

US-CL-CURRENT: 435/220; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

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☐ 15. Document ID: US 20050221459 A1

L9: Entry 15 of 101 File: PGPB Oct 6, 2005

PGPUB-DOCUMENT-NUMBER: 20050221459
PGPUB-FILING-TYPE: new

DOCUMENT-IDENTIFIER: US 20050221459 A1

TITLE: Geranylgeranyl transferase type I (GGTase-I) structure and uses thereof

PUBLICATION-DATE: October 6, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Taylor, Jeffrey S.	Milford	CT	US
Reid, T. Scott	Durham	NC	US
Beese, Lorena S.	Durham	NC	US

US-CL-CURRENT: 435/193; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw D

☐ 16. Document ID: US 20050215795 A1

L9: Entry 16 of 101 File: PGPB Sep 29, 2005

PGPUB-DOCUMENT-NUMBER: 20050215795
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050215795 A1

TITLE: Process for preparing 2-aminothiazole-5-aromatic carboxamides as kinase inhibitors

PUBLICATION-DATE: September 29, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Chen, Bang-Chi	Plainsboro	NJ	US
Droghini, Roberto	Candiac	NJ	CA
Lajeunesse, Jean	Candiac	NJ	CA
Dimarco, John D.	East Brunswick	NJ	US
Galella, Michael	Kendall Park		US
Chidambaram, Ramakrishnan	Pennington		US

US-CL-CURRENT: 548/190

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw D

☐ 17. Document ID: US 20050215477 A1

L9: Entry 17 of 101 File: PGPB Sep 29, 2005

PGPUB-DOCUMENT-NUMBER: 20050215477
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050215477 A1

TITLE: Crystallization of IGF-1

PUBLICATION-DATE: September 29, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Schaffer, Michelle	Cambridge	CA	GB
Ultsch, Mark	Mill Valley	CT	US
Vajdos, Felix	Ledyard		US

US-CL-CURRENT: 514/12; 530/399, 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw D

☐ 18. Document ID: US 20050214918 A1

L9: Entry 18 of 101 File: PGPB Sep 29, 2005

PGPUB-DOCUMENT-NUMBER: 20050214918
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050214918 A1

TITLE: Novel purified polypeptides from streptococcus pneumoniae

PUBLICATION-DATE: September 29, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Edwards, Aled	Toronto		CA
Dharamsi, Akil	Richmond Hill		CA
Vedadi, Masoud	Toronto		CA
Kimber, Matthew	Toronto		CA

US-CL-CURRENT: 435/193; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw D

☐ 19. Document ID: US 20050214773 A1

L9: Entry 19 of 101 File: PGPB Sep 29, 2005

PGPUB-DOCUMENT-NUMBER: 20050214773
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050214773 A1

TITLE: Novel purified polypeptides from bacteria

PUBLICATION-DATE: September 29, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Edwards, Aled	Toronto		CA
Dharamsi, Akil	Richmond Hill		CA
Vedadi, Masoud	Toronto		CA
Alam, Muhammad Zahoor	Oshawa		CA
Domagala, Megan	Woodstock		CA
Houston, Simon	Toronto		CA
Lam, Robert	Toronto		CA
Li, Qin	Toronto		CA
Nethery-Brokx, Kathleen	Toronto		CA
Ng, Ivy	Toronto		CA
Pinder, Benjamin	Toronto		CA
Viola, Cristina	Caledon		CA
Wrezel, Olga	Mississauga		CA
Kanagarajah, Dhushy	Mississauga		CA
Mansoury, Kamran	Toronto		CA
Necakov, Sasha Aleksandar	Toronto		CA
Vallee, Francois	Toronto		CA
McDonald, Merry-Lynn	Ajax		CA

US-CL-CURRENT: 435/6; 435/193, 435/252.3, 435/320.1, 435/69.1, 536/23.2

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. D

☐ 20. Document ID: US 20050187718 A1

L9: Entry 20 of 101 File: PGPB Aug 25, 2005

PGPUB-DOCUMENT-NUMBER: 20050187718
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050187718 A1

TITLE: Novel purified polypeptides from Streptococcus pneumoniae

PUBLICATION-DATE: August 25, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Edwards, Aled	Toronto	NY	CA
Dharamsi, Akil	Richmond Hill		CA
Vedadi, Masoud	Toronto		CA
Clarke, Teresa	Toronto		CA
Kimber, Matthew	Toronto		CA
Sharma, Vivek	Buffalo		US
Houston, Simon	Toronto		CA
Mansoury, Kamran	Toronto		CA

US-CL-CURRENT: 702/19; 435/183

☐ 21. Document ID: US 20050186636 A1

L9: Entry 21 of 101 File: PGPB Aug 25, 2005

PGPUB-DOCUMENT-NUMBER: 20050186636
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050186636 A1

TITLE: Method of rational-based drug design using osteocalcin

PUBLICATION-DATE: August 25, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Yang, Daniel S.C.	Dundas		CA
Hoang, Quyen	Brantford		CA

US-CL-CURRENT: 435/7.1; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw. D

☐ 22. Document ID: US 20050181464 A1

L9: Entry 22 of 101 File: PGPB Aug 18, 2005

PGPUB-DOCUMENT-NUMBER: 20050181464
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050181464 A1

TITLE: Novel purified polypeptides from bacteria

PUBLICATION-DATE: August 18, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Edwards, Aled	Toronto		CA
Dharamsi, Akil	Richmond Hill		CA
Vedadi, Masoud	Toronto		CA
Alam, Muhammad Zahoor	Oshawa		CA
Arrowsmith, Cheryl	Toronto		CA
Awrey, Donald E.	Mississauga		CA
Beattie, Bryan	Oakville		CA
Buzadzija, Kristina	Mississauga		CA
Clarke, Teresa	Toronto		CA
Domagala, Megan	Woodstock		CA
Houston, Simon	Toronto		CA
Kanagarajah, Dhushy	Mississauga		CA

Li, Qin	Toronto	CA
Mansoury, Kamran	Toronto	CA
McDonald, Merry-Lynn	Ajax	CA
Nethery-Brokx, Kathleen	Toronto	CA
Ng, Ivy	Toronto	CA
Ouyang, Hui	Toronto	CA
Richards, Dawn	Toronto	CA
Vallee, Francois	Toronto	CA
Virag, Cristina	Brampton	CA

US-CL-CURRENT: 435/7.32; 436/86, 530/350

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw De

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☐ 23. Document ID: US 20050181388 A1

L9: Entry 23 of 101 File: PGPB Aug 18, 2005

PGPUB-DOCUMENT-NUMBER: 20050181388
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050181388 A1

TITLE: Novel purified polypeptides from bacteria

PUBLICATION-DATE: August 18, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Edwards, Aled	Toronto		CA
Dharamsi, Akil	Richmond Hill		CA
Vedadi, Masoud	Toronto		CA
Alam, Muhammad Zahoor	Oshawa		CA
Arrowsmith, Cheryl	Toronto		CA
Awrey, Donald E.	Mississauga		CA
Beattie, Bryan	Oakville		CA
Buzadzija, Kristina	Mississauga		CA
Canadien, Veronica	Toronto		CA
Domagala, Megan	Woodstock		CA
Houston, Simon	Toronto		CA
Kanagarajah, Dhushy	Mississauga		CA
Li, Qin	Toronto		CA
Mansoury, Kamran	Toronto		CA
McDonald, Merry-Lynn	Ajax		CA
Nethery-Brokx, Kathleen	Toronto		CA
Ng, Ivy	Toronto		CA
Ouyang, Hui	Toronto		CA
Pinder, Benjamin	Toronto		CA
Richards, Dawn	Toronto		CA

Tai, Matthew	Toronto	CA
Thalakada, Rosanne	St. Catherines	CA
Vallee, Francois	Toronto	CA
Virag, Cristina	Brampton	CA

US-CL-CURRENT: 435/6; 436/86

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw De

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☐ 24. Document ID: US 20050181362 A1

L9: Entry 24 of 101 File: PGPB Aug 18, 2005

PGPUB-DOCUMENT-NUMBER: 20050181362
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050181362 A1

TITLE: Crystallized glucocorticoid receptor ligand binding domain polypeptide and screening methods employing same

PUBLICATION-DATE: August 18, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Apolito, Christopher J.	Durham	NC	US
Bledsoe, Randy K.	Durham	NC	US
Lambert III, Millard H.	Durham	NC	US
McKee, David D.	Durham	NC	US
Montana, Valerie Gail	Durham	NC	US
Pearce, Kenneth H.	Durham	NC	US
Stanley, Thomas B.	Durham	NC	US
Xu, Huaqiang Eric	Grand Rapids	MI	US
Delves, Christopher J.	Stevenage		GB

US-CL-CURRENT: 435/6; 435/199, 435/252.3, 435/69.1, 435/7.1, 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw De

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☐ 25. Document ID: US 20050170431 A1

L9: Entry 25 of 101 File: PGPB Aug 4, 2005

PGPUB-DOCUMENT-NUMBER: 20050170431
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050170431 A1

TITLE: PYK2 crystal structure and uses

PUBLICATION-DATE: August 4, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Ibrahim, Prabha	Mountain View	CA	US
Krupka, Heike	Hayward	CA	US
Kumar, Abhinav	Pleasant Hill	CA	US
Milburn, Michael V.	Emeryville	CA	US
Suzuki, Yoshihisa	El Sobrante	CA	US

US-CL-CURRENT: 435/7.1; 530/388.26

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw De

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☐ 26. Document ID: US 20050165218 A1

L9: Entry 26 of 101 File: PGPB Jul 28, 2005

PGPUB-DOCUMENT-NUMBER: 20050165218
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050165218 A1

TITLE: Crystal structure of the ligand binding domain of the retinoic acid-related orphan receptor alpha (ror-alpha)

PUBLICATION-DATE: July 28, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Beerli, Rene	Binningen		CH
Fournier, Brigitte	Riedisheim		FR
Kallen, Jorg	Basel		CH
Schlaeppi, Jean-Marc	Allschwil		CH

US-CL-CURRENT: 530/350; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw De

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☐ 27. Document ID: US 20050164363 A1

L9: Entry 27 of 101 File: PGPB Jul 28, 2005

PGPUB-DOCUMENT-NUMBER: 20050164363
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050164363 A1

TITLE: Novel purified polypeptides from staphylococcus aureus

PUBLICATION-DATE: July 28, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY

Edwards, Aled	Toronto	CA
Dharamsi, Akil	Richmond Hill	CA
Vedadi, Masoud	Toronto	CA
Houston, Simon	Toronto	CA
Kimber, Matthew	Toronto	CA

US-CL-CURRENT: 435/193; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw. De

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☐ 28. Document ID: US 20050164362 A1

L9: Entry 28 of 101 File: PGPB Jul 28, 2005

PGPUB-DOCUMENT-NUMBER: 20050164362
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050164362 A1

TITLE: Novel purified polypeptides from pseudomonas aeruginosa

PUBLICATION-DATE: July 28, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Edwards, Aled	Toronto		CA
Dharamsi, Akil	Richmond Hill		CA
Vedadi, Masoud	Toronto		CA
Alam, Muhammad Zahoor	Oshawa		CA
Domagala, Megan	Woodstock		CA
Houston, Simon	Toronto		CA
Kimber, Matthew	Toronto		CA
Pinder, Benjamin	Toronto		CA
Vallee, Francois	Toronto		CA
Wrezel, Olga	Mississauga		CA
Awrey, Donald E.	Mississauga		CA
Beattie, Bryan	Oakville		CA

US-CL-CURRENT: 435/183; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw. De

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☐ 29. Document ID: US 20050164300 A1

L9: Entry 29 of 101 File: PGPB Jul 28, 2005

PGPUB-DOCUMENT-NUMBER: 20050164300
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050164300 A1

TITLE: Molecular scaffolds for kinase ligand development

PUBLICATION-DATE: July 28, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Artis, Dean R.	Kensington	CA	US
Bremer, Ryan E.	Oakland	CA	US
Gillette, Samuel J.	Oakland	CA	US
Hurt, Clarence R.	San Ramon	CA	US
Ibrahim, Prabha L.	Mountain View	CA	US
Zuckerman, Rebecca L.	Alameda	CA	US

US-CL-CURRENT: 435/7.1; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw D

☐ 30. Document ID: US 20050158732 A1

L9: Entry 30 of 101 File: PGPB Jul 21, 2005

PGPUB-DOCUMENT-NUMBER: 20050158732
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050158732 A1

TITLE: Novel purified polypeptides from Streptococcus pneumoniae

PUBLICATION-DATE: July 21, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Edwards, Aled	Toronto		CA
Dharamsi, Akil	Richmond Hill		CA
Vedadi, Masoud	Toronto		CA
Alam, Muhammad Zahoor	Oshawa		CA
Houston, Simon	Toronto		CA
Kimber, Matthew	Toronto		CA
Lam, Robert	Toronto		CA
Ng, Ivy	Toronto		CA
Pinder, Benjamin	Toronto		CA

US-CL-CURRENT: 435/6; 435/191, 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw D

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☐ 31. Document ID: US 20050107298 A1

L9: Entry 31 of 101 File: PGPB May 19, 2005

PGPUB-DOCUMENT-NUMBER: 20050107298
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050107298 A1

TITLE: Crystals and structures of c-Abl tyrosine kinase domain

PUBLICATION-DATE: May 19, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Louie, Gordon V.	San Diego	CA	US
Buchanan, Sean Grant	Encinitas	CA	US
Chie Leon, Barbara	Chula Vista	CA	US
Arnold, William D.	San Diego	CA	US

US-CL-CURRENT: 514/12; 530/350, 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw D

☐ 32. Document ID: US 20050048573 A1

L9: Entry 32 of 101 File: PGPB Mar 3, 2005

PGPUB-DOCUMENT-NUMBER: 20050048573
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050048573 A1

TITLE: PDE5A crystal structure and uses

PUBLICATION-DATE: March 3, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Artis, Dean R.	Kensington	CA	US
Bollag, Gideon	Orinda	CA	US
Card, Graeme	Oakland	CA	US
Martin, Fernando	Toronto	NC	CA
Milburn, Michael V.	Cary	CA	US

Zhang, Kam Walnut Creek US

US-CL-CURRENT: 435/7.1; 436/518

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw De

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☐ 33. Document ID: US 20050038611 A1

L9: Entry 33 of 101 File: PGPB Feb 17, 2005

PGPUB-DOCUMENT-NUMBER: 20050038611
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050038611 A1

TITLE: S8 rrna-binding protein from the small ribosomal subunit of staphylococcus aureus

PUBLICATION-DATE: February 17, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Concha, Nestor O.	King of Prussia	PA	US
Gontarek, Richard K	King of Prussia	PA	US
Janson, Cheryl A	Hinsdale	IL	US

US-CL-CURRENT: 702/20; 435/6, 530/358

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw De

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☐ 34. Document ID: US 20050037478 A1

L9: Entry 34 of 101 File: PGPB Feb 17, 2005

PGPUB-DOCUMENT-NUMBER: 20050037478
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050037478 A1

TITLE: Crystal structure of glutamate racemase (MurI)

PUBLICATION-DATE: February 17, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Anderson, Marie	Lindome	MA	SE
Fisher, Stewart Lindsay	Framingham	MA	US
Folmer, Rutger Henk Adriaan	Lindome		SE
Kern, Gunther	Waltham		US
Lundqvist, Rolf Tomas	Gothenburg		SE
Newton, David Trevor	Ottawa		CA
Xue, Yafeng	Askim		SE

US-CL-CURRENT: 435/233; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

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☐ 35. Document ID: US 20050037476 A1

L9: Entry 35 of 101 File: PGPB Feb 17, 2005

PGPUB-DOCUMENT-NUMBER: 20050037476
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050037476 A1

TITLE: Modified Wee1, crystals of peptide: inhibitor complexes containing such modified Wee1, and methods of use thereof

PUBLICATION-DATE: February 17, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Baker, Edward Neill	Takapuna	MI	NZ
Booth, Richard John	Ann Arbor	MI	US
Kraker, Alan J.	Ann Arbor	MI	US
Ortwine, Daniel Fred	Saline		US
Dickson, James Michael Jeremy	Beachhaven		NZ
Ivanovic, Ivan	Ellerslie		NZ
Squire, Christopher John	Devonport		NZ

US-CL-CURRENT: 435/184; 435/199, 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

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☐ 36. Document ID: US 20050036997 A1

L9: Entry 36 of 101 File: PGPB Feb 17, 2005

PGPUB-DOCUMENT-NUMBER: 20050036997
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050036997 A1

TITLE: RIBOSOME STRUCTURE AND PROTEIN SYNTHESIS INHIBITORS

PUBLICATION-DATE: February 17, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Steitz, Thomas A.	Branford	CT	US
Moore, Peter B.	North Haven	CT	US
Sutcliffe, Joyce A.	Clinton	CT	US
Oyelere, Adegboyega K.	New Haven	CT	US
Ippolito, Joseph A.	Guilford	CT	US

US-CL-CURRENT: 424/94.1; 435/184, 514/28

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

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☐ 37. Document ID: US 20050033035 A1

L9: Entry 37 of 101 File: PGPB Feb 10, 2005

PGPUB-DOCUMENT-NUMBER: 20050033035
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20050033035 A1

TITLE: Mutants of igf binding proteins and methods of production of antagonists thereof

PUBLICATION-DATE: February 10, 2005

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Beisel, Hans-Georg	Molndal		DE
Demuth, Dirk	Munster-Sarmsheim		DE
Engh, Richard	Wessling		DE
Holak, Tadeusz	Martinsried		DE
Huber, Robert	Germering		DE
Lang, Kurt	Penzberg		DE
Schumacher, Ralf	Penzberg		DE
Zeslawski, Wojciech	Krakow		PL

US-CL-CURRENT: 530/399; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

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☐ 38. Document ID: US 20040265983 A1

L9: Entry 38 of 101 File: PGPB Dec 30, 2004

PGPUB-DOCUMENT-NUMBER: 20040265983
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20040265983 A1

TITLE: Crystalline TNF-alpha-converting enzyme and uses thereof

PUBLICATION-DATE: December 30, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Black, Roy A.	Seattle	WA	US
Paxton, Raymond James	Bellevue	WA	US
Bode, Wolfram	Gauting	NJ	DE
Maskos, Klaus	Holzkirchem	NY	DE

Fernandez-Catalan, Carlos	Martinsried-Planegg	DE
Chen, James Ming	Bedminster	US
Levin, Jeremy Ian	New York	US

US-CL-CURRENT: 435/226; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw De

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☐ 39. Document ID: US 20040259945 A1

L9: Entry 39 of 101 File: PGPB Dec 23, 2004

PGPUB-DOCUMENT-NUMBER: 20040259945
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20040259945 A1

TITLE: Tetrapropylammonium tetrathiomolybdate and related compounds for anti-angiogenic therapies

PUBLICATION-DATE: December 23, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Brewer, George J.	Ann Arbor	MI	US
Merajver, Sofia D.	Ann Arbor	MI	US
Coucouvanis, Dimitri	Ann Arbor	MI	US

US-CL-CURRENT: 514/492

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw De

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☐ 40. Document ID: US 20040253178 A1

L9: Entry 40 of 101 File: PGPB Dec 16, 2004

PGPUB-DOCUMENT-NUMBER: 20040253178
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20040253178 A1

TITLE: Crystals and structures of spleen tyrosine kinase SYKKD

PUBLICATION-DATE: December 16, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Atwell, Shane	Encinitas	CA	US
Hendle, Jorg	San Diego	CA	US
Buchanan, Sean Grant	Encinitas	CA	US
Feil, Ingeborg	San Diego	CA	US
Russell, Marijane	Solana Beach	CA	US

Badger, John	San Diego	CA	US
Tomimoto, Masaki	San Diego	CA	US
Sauder, Michael J.	Carlsbad	CA	US

US-CL-CURRENT: 424/1.69; 530/350, 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw De

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☐ 41. Document ID: US 20040248800 A1

L9: Entry 41 of 101 File: PGPB Dec 9, 2004

PGPUB-DOCUMENT-NUMBER: 20040248800
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20040248800 A1

TITLE: Crystals and structures of epidermal growth factor receptor kinase domain

PUBLICATION-DATE: December 9, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Atwell, Shane	San Diego	CA	US
Buchanan, Sean Grant	Encinitas	CA	US

US-CL-CURRENT: 514/12; 435/7.1, 530/350, 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw De

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☐ 42. Document ID: US 20040243316 A1

L9: Entry 42 of 101 File: PGPB Dec 2, 2004

PGPUB-DOCUMENT-NUMBER: 20040243316
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20040243316 A1

TITLE: Crystallographic structure of the androgen receptor ligand binding domain

PUBLICATION-DATE: December 2, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Weinmann, Roberto	Lawrenceville	NJ	US
Einspahr, Howard M.	Lawrenceville	NJ	US
Krystek, Stanley R.	Ringoes	NJ	US
Sack, John S.	Lawrenceville	NJ	US
Salvati, Mark E.	Lawrenceville	NJ	US
Tokarski, John S.	Princeton	NJ	US

Attar, Ricardo M.	Lawrenceville	NJ	US
Wang, Chihuei	Plainsboro	NJ	US

US-CL-CURRENT: 702/19; 435/7.1, 530/350

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

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☐ 43. Document ID: US 20040229792 A1

L9: Entry 43 of 101 File: PGPB Nov 18, 2004

PGPUB-DOCUMENT-NUMBER: 20040229792
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20040229792 A1

TITLE: Peripheral nervous system specific sodium channels, DNA encoding therefor, crystallization, X-ray diffraction, computer molecular modeling, rational drug design, drug screening, and methods of making and using thereof

PUBLICATION-DATE: November 18, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Mandel, Gail	Stony Brook	NY	US
Halegoua, Simon	Belle Terre	NY	US

US-CL-CURRENT: 514/12; 435/6, 514/317

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

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☐ 44. Document ID: US 20040219653 A1

L9: Entry 44 of 101 File: PGPB Nov 4, 2004

PGPUB-DOCUMENT-NUMBER: 20040219653
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20040219653 A1

TITLE: Crystal structure of homo sapiens adipocyte lipid binbing protein and uses thereof

PUBLICATION-DATE: November 4, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Qiu, Xiayang	Mystic	CT	US

US-CL-CURRENT: 435/198; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

☐ 45. Document ID: US 20040209344 A1

L9: Entry 45 of 101 File: PGPB Oct 21, 2004

PGPUB-DOCUMENT-NUMBER: 20040209344
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20040209344 A1

TITLE: Crystal structure of angiotensin-converting enzyme-related carboxypeptidase

PUBLICATION-DATE: October 21, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Pantoliano, Michael W.	Boxford	MA	US
Ryan, M. Dominic	Littleton	MA	US
Staker, Bart Lee	Kingston	WA	US
Prasad, G. Sridhar	San Diego	CA	US
Tang, Jin	Canton	MA	US
Menon, Saurabh Prabhakar	Medford	MA	US
Towler, Paul S.	Gloucester	MA	US
Williams, David H.	London		GB
Fisher, Martin	Wakefield		GB

US-CL-CURRENT: 435/226; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

☐ 46. Document ID: US 20040171062 A1

L9: Entry 46 of 101 File: PGPB Sep 2, 2004

PGPUB-DOCUMENT-NUMBER: 20040171062
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20040171062 A1

TITLE: Methods for the design of molecular scaffolds and ligands

PUBLICATION-DATE: September 2, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Hirth, Klaus-Peter	San Francisco	CA	US
Milburn, Michael Vance	Emeryville	CA	US

US-CL-CURRENT: 435/7.1; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

☐ 47. Document ID: US 20040157309 A1

L9: Entry 47 of 101 File: PGPB Aug 12, 2004

PGPUB-DOCUMENT-NUMBER: 20040157309
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20040157309 A1

TITLE: Crystalline form of the catalytic domain of ADAM33 and methods of use thereof

PUBLICATION-DATE: August 12, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Orth, Peter	New York City	NY	US
Reichert, Paul	Montville	NJ	US
Madison, Vincent S.	Mountain Lakes	NY	US
Wang, Wenyan	Edison	NJ	US
Zou, Jun	Cranbury	NJ	US

US-CL-CURRENT: 435/226; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw D

☐ 48. Document ID: US 20040151715 A1

L9: Entry 48 of 101 File: PGPB Aug 5, 2004

PGPUB-DOCUMENT-NUMBER: 20040151715
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20040151715 A1

TITLE: Catalytic domain of ADAM33 and methods of use thereof

PUBLICATION-DATE: August 5, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Wang, Wenyan	Edison	NJ	US
Le, Hung V.	Rockaway	NJ	US
Liu, Jian-Jun	Parlin	NJ	US
Madison, Vincent S.	Mountain Lakes	NJ	US
Prosise, Winifred W.	Ramsey	NJ	US
Taremi, Shahriar Shane	Upper Montclair	NJ	US
Xiao, Li	Woodbridge	NJ	US
Zou, Jun	Cranbury	NJ	US

US-CL-CURRENT: 424/94.63; 435/226, 435/7.1

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

☐ 49. Document ID: US 20040142864 A1

L9: Entry 49 of 101 File: PGPB Jul 22, 2004

PGPUB-DOCUMENT-NUMBER: 20040142864
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20040142864 A1

TITLE: Crystal structure of PIM-1 kinase

PUBLICATION-DATE: July 22, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Bremer, Ryan	Oakland	CA	US
Ibrahim, Prabha	Mountain View	CA	US
Kumar, Abhinav	Pleasant Hill	CA	US
Mandiyan, Valsan	Bloomfield	NJ	US
Milburn, Michael V.	Emeryville	CA	US

US-CL-CURRENT: 514/12; 435/7.1

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

☐ 50. Document ID: US 20040133356 A1

L9: Entry 50 of 101 File: PGPB Jul 8, 2004

PGPUB-DOCUMENT-NUMBER: 20040133356
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20040133356 A1

TITLE: Three-dimensional model of a Fc region of an IgE antibody and uses thereof

PUBLICATION-DATE: July 8, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Jardetzky, Theodore S.	Chicago	IL	US
Wurzburg, Beth A.	Evanston	IL	US

US-CL-CURRENT: 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

☐ 51. Document ID: US 20040081651 A1

L9: Entry 51 of 101 File: PGPB Apr 29, 2004

PGPUB-DOCUMENT-NUMBER: 20040081651
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20040081651 A1

TITLE: Antibodies to vla-1

PUBLICATION-DATE: April 29, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Karpusas, Michael	Upper Darby	PA	US
Lyne, Paul D	Arlington	MA	US
Saldanha, Jose William B	Middlesex	MA	GB
Garber, Ellen A	Cambridge		US

US-CL-CURRENT: 424/146.1

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

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☐ 52. Document ID: US 20040063951 A1

L9: Entry 52 of 101 File: PGPB Apr 1, 2004

PGPUB-DOCUMENT-NUMBER: 20040063951
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20040063951 A1

TITLE: Alkaloid halide salts of swainsonine and methods of use

PUBLICATION-DATE: April 1, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Dennis, James W.	Etobicoke		CA
Shah, Rajan N.	Toronto		CA
Ziser, Lothar	Toronto		CA

US-CL-CURRENT: 546/136

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

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☐ 53. Document ID: US 20040063666 A1

L9: Entry 53 of 101 File: PGPB Apr 1, 2004

PGPUB-DOCUMENT-NUMBER: 20040063666
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20040063666 A1

TITLE: Compositions for inhibiting arginase activity

PUBLICATION-DATE: April 1, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Christianson, David	Media	PA	US
Baggio, Ricky	Waltham	MA	US
Elbaum, Daniel	Newton	MA	US

US-CL-CURRENT: 514/64

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

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☐ 54. Document ID: US 20040058425 A1

L9: Entry 54 of 101 File: PGPB Mar 25, 2004

PGPUB-DOCUMENT-NUMBER: 20040058425
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20040058425 A1

TITLE: Crystal structure

PUBLICATION-DATE: March 25, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Knoechel, Thorsten Reginald	Sandwich		GB
Robinson, Colin Mark	Sandwich		GB
Taylor, Wendy Elaine	Sandwich		GB
Tucker, Alexander Dunbar	Sandwich		GB

US-CL-CURRENT: 435/194; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

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☐ 55. Document ID: US 20040054480 A1

L9: Entry 55 of 101 File: PGPB Mar 18, 2004

PGPUB-DOCUMENT-NUMBER: 20040054480
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20040054480 A1

TITLE: Three dimensional structures and models of Fc receptors and uses thereof

PUBLICATION-DATE: March 18, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Hogarth, P. Mark	Williamstown		AU
Powell, Maree S.	Ferntree Gully		AU
McKenzie, Ian F.C.	Brunswick		AU
Maxwell, Kelly F.	South Yarra		AU
Garrett, Thomas P.J.	Brunswick		AU
Epa, Vidana	Parkville		AU

US-CL-CURRENT: 702/19; 702/27, 703/11

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. D

☐ 56. Document ID: US 20040033527 A1

L9: Entry 56 of 101 File: PGPB Feb 19, 2004

PGPUB-DOCUMENT-NUMBER: 20040033527
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20040033527 A1

TITLE: Methods of using a three-dimensional model of a Fc epsilon receptor alpha chain

PUBLICATION-DATE: February 19, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Jardetzky, Theodore S.	Chicago	IL	US
Garman, Scott Clayton	Evanston	IL	US
Kinet, Jean-Pierre	Lexington	MA	US

US-CL-CURRENT: 435/7.1; 703/11

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. D

☐ 57. Document ID: US 20040029129 A1

L9: Entry 57 of 101 File: PGPB Feb 12, 2004

PGPUB-DOCUMENT-NUMBER: 20040029129
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20040029129 A1

TITLE: Identification of essential genes in microorganisms

PUBLICATION-DATE: February 12, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Wang, Liangsu	San Diego	CA	US

Zamudio, Carlos	La Jolla	CA	US
Malone, Cheryl	Santee	CA	US
Haselbeck, Robert	San Diego	CA	US
Ohlsen, kari L.	San Diego	CA	US
Zyskind, Judith W.	La Jolla	CA	US
Wall, Daniel	San Diego	CA	US
Trawick, John D.	La Mesa	CA	US
Carr, Grant J.	Escondido	CA	US
Yamamoto, Robert	San Diego	CA	US
Forsyth, R. Allyn	San Diego	CA	US
Xu, H. Howard	San Diego	CA	US

US-CL-CURRENT: 435/6; 435/183, 435/252.33, 435/254.2, 435/320.1, 435/325, 435/419, 435/69.1, 530/350, 536/23.2

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

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☐ 58. Document ID: US 20040018560 A1

L9: Entry 58 of 101 File: PGPB Jan 29, 2004

PGPUB-DOCUMENT-NUMBER: 20040018560
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20040018560 A1

TITLE: Crystallized LXR polypeptide in complex with a ligand and screening methods employing same

PUBLICATION-DATE: January 29, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Bledsoe, Randy K.	Durham	NC	US
Miller, Ann	Wilmington	NC	US
Moore, John T.	Durham	NC	US
Moore, Linda	Durham	NC	US
Williams, Shawn P.	Durham	NC	US
Wisely, George B.	Durham	NC	US

US-CL-CURRENT: 435/7.1; 530/350, 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

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☐ 59. Document ID: US 20040018558 A1

L9: Entry 59 of 101 File: PGPB Jan 29, 2004

PGPUB-DOCUMENT-NUMBER: 20040018558
PGPUB-FILING-TYPE: new

DOCUMENT-IDENTIFIER: US 20040018558 A1

TITLE: Method for identifying modulators of G protein coupled receptor signaling

PUBLICATION-DATE: January 29, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Gilchrist, Annette	Barrington	IL	US
Hamm, Heidi M.	Nashville	TN	US

US-CL-CURRENT: 435/7.1; 436/518

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw D

☐ 60. Document ID: US 20040014948 A1

L9: Entry 60 of 101 File: PGPB Jan 22, 2004

PGPUB-DOCUMENT-NUMBER: 20040014948
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20040014948 A1

TITLE: Single-chain antagonist polypeptides

PUBLICATION-DATE: January 22, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Halkier, Torben	Solroed Strand	CA	DK
Schambye, Hans Thalsgard	Holte		DK
Okkels, Jens Sigurd	Vedbaek		DK
Andersen, Kim Vilbour	Broenshoej		DK
Nissen, Torben Lauesgaard	San Francisco		US
Soni, Bobby	Copenhagen K.		DK
Jeppesen, Claus Bekker	Nivaa		DK
van den Hazel, Bart	Copenhagen		DK

US-CL-CURRENT: 530/388.22; 530/324

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw D

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☐ 61. Document ID: US 20040014194 A1

L9: Entry 61 of 101 File: PGPB Jan 22, 2004

PGPUB-DOCUMENT-NUMBER: 20040014194
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20040014194 A1

TITLE: Beta-secretase crystals and methods for preparing and using the same

PUBLICATION-DATE: January 22, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Beyer, Brian M.	Lincroft	NJ	US
Hammond, Gerald S.	Newark	NJ	US
Reichert, Paul	Montville	NJ	US
Strickland, Corey	Martinsville	NJ	US
Wang, Wenyan	Edison	NJ	US
Weber, Patricia C.	Yardley	PA	US
Wong, Gwendolyn Tse	Westfield	NJ	US
Zhang, Lili	Scotch Plains	NJ	US

US-CL-CURRENT: 435/226; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw D

☐ 62. Document ID: US 20040009569 A1

L9: Entry 62 of 101 File: PGPB Jan 15, 2004

PGPUB-DOCUMENT-NUMBER: 20040009569
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20040009569 A1

TITLE: Kinase crystal structures and materials and methods for kinase activation

PUBLICATION-DATE: January 15, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Barford, David	London		GB

Yang, Jing	Middlesex	GB
Hemmings, Brian Arthur	Bettingen	CH
Cron, Peter David	Basel	CH

US-CL-CURRENT: 435/194; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

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☐ 63. Document ID: US 20040006208 A1

L9: Entry 63 of 101 File: PGPB Jan 8, 2004

PGPUB-DOCUMENT-NUMBER: 20040006208
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20040006208 A1

TITLE: Co-crystal structure of monoclonal antibody 5C8 and CD154, and use thereof in drug design

PUBLICATION-DATE: January 8, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Karpusas, Michael	Upper Darby	PA	US
Hsu, Yen-Ming	Lexington	MA	US
Taylor, Frederick R.	Milton	MA	US
Zheng, Zhongli	Lexington	MA	US

US-CL-CURRENT: 530/350; 530/388.22, 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

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☐ 64. Document ID: US 20040005687 A1

L9: Entry 64 of 101 File: PGPB Jan 8, 2004

PGPUB-DOCUMENT-NUMBER: 20040005687
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20040005687 A1

TITLE: Kinase crystal structures

PUBLICATION-DATE: January 8, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Barford, David	London		GB
Yang, Jing	Middlesex		GB
Hemmings, Brian Arthur	Bettingen		CH
Cron, Peter David	Basel		CH

US-CL-CURRENT: 435/194; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

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☐ 65. Document ID: US 20040002586 A1

L9: Entry 65 of 101 File: PGPB Jan 1, 2004

PGPUB-DOCUMENT-NUMBER: 20040002586
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20040002586 A1

TITLE: Crystal structure of interleukin-22 and uses thereof

PUBLICATION-DATE: January 1, 2004

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Nagem, Ronaldo A.P.	Campinas		BR
Polikarpov, Igor	San Carlos		BR
Renauld, Jean Christophe	Brussels		BE
Colau, Didier	Brussels		BE
Dumoutier, Laure	Brussels		BE

US-CL-CURRENT: 530/351; 703/11

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

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☐ 66. Document ID: US 20030232779 A1

L9: Entry 66 of 101 File: PGPB Dec 18, 2003

PGPUB-DOCUMENT-NUMBER: 20030232779
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20030232779 A1

TITLE: Determination and uses of the atomic structures of ribosomes and ribosomal subunits and their ligand complexes

PUBLICATION-DATE: December 18, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Steitz, Thomas A.	Branford	CT	US
Moore, Peter B.	North Haven	CT	US
Ban, Nenad	Zurich	CT	CH
Nissen, Poul	Aarhus N		DK
Hansen, Jeffrey	New Haven		US

US-CL-CURRENT: 514/44; 435/317.1, 702/20

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw De

☐ 67. Document ID: US 20030225527 A1

L9: Entry 67 of 101 File: PGPB Dec 4, 2003

PGPUB-DOCUMENT-NUMBER: 20030225527
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20030225527 A1

TITLE: Crystals and structures of MST3

PUBLICATION-DATE: December 4, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Antonysamy, Stephen Suresh	San Diego	CA	US
Feil, Ingeborg	San Diego	CA	US
Buchanan, Sean Grant	Encinitas	CA	US
Xu, Jian	San Diego	CA	US

US-CL-CURRENT: 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw De

☐ 68. Document ID: US 20030224500 A1

L9: Entry 68 of 101 File: PGPB Dec 4, 2003

PGPUB-DOCUMENT-NUMBER: 20030224500
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20030224500 A1

TITLE: Modified MEK1 and MEK2, crystal of a peptide: ligand: cofactor complex containing such modified MEK1 or MEK2, and methods of use thereof

PUBLICATION-DATE: December 4, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Ohren, Jeffrey F.	Saline	MI	US
Chen, Huifen	Plymouth	MI	US
Delaney, Amy Marie	Belleville	MI	US
Dudley, David Thomas	Ann Arbor	MI	US
Hasemann, Charles A. JR.	Williamston	MI	US
Kuffa, Peter	Ann Arbor	MI	US
McConnell, Patrick C.	Ann Arbor	MI	US
Pavlovsky, Alexander Gregory	Ann Arbor	MI	US

Tecle, Haile	Ann Arbor	MI	US
Whitehead, Christopher E.	Ypsilanti	MI	US
Yan, Chunhong	Ann Arbor	MI	US
Zhang, Erli	Canton	MI	US

US-CL-CURRENT: 435/194; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw De

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☐ 69. Document ID: US 20030224468 A1

L9: Entry 69 of 101 File: PGPB Dec 4, 2003

PGPUB-DOCUMENT-NUMBER: 20030224468
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20030224468 A1

TITLE: Treatment or prophylaxis of diseases caused by pilus-forming bacteria

PUBLICATION-DATE: December 4, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Hultgren, Scott	Ballwin	MO	US
Kuehn, Meta	Berkeley	CA	US
Xu, Zheng	Blue Bell	PA	US
Ogg, Derek	Uppsala	MO	SE
Harris, Mark	Uppsala		SE
Lepisto, Matti	Lund		SE
Jones, Charles Hal	Saint Louis		US
Kihlberg, Jan	Dalby		SE

US-CL-CURRENT: 435/7.32; 514/110, 514/327, 514/42, 536/18.7, 536/4.1, 546/242

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw De

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☐ 70. Document ID: US 20030224335 A1

L9: Entry 70 of 101 File: PGPB Dec 4, 2003

PGPUB-DOCUMENT-NUMBER: 20030224335
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20030224335 A1

TITLE: Receptor linked protein tyrosine phosphatases

PUBLICATION-DATE: December 4, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Frederick, Christin	Newton	MA	US
Saito, Haruo	Newton	MA	US

US-CL-CURRENT: 434/193; 436/86

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

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☐ 71. Document ID: US 20030215874 A1

L9: Entry 71 of 101 File: PGPB Nov 20, 2003

PGPUB-DOCUMENT-NUMBER: 20030215874
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20030215874 A1

TITLE: Isolated GRP94 ligand binding domain polypeptide and nucleic acid encoding same, crystalline form of same, and screening methods employing same

PUBLICATION-DATE: November 20, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Gewirth, Daniel T.	Durham	NC	US
Nicchitta, Christopher V.	Durham	NC	US

US-CL-CURRENT: 435/7.1; 435/189, 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

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☐ 72. Document ID: US 20030211538 A1

L9: Entry 72 of 101 File: PGPB Nov 13, 2003

PGPUB-DOCUMENT-NUMBER: 20030211538
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20030211538 A1

TITLE: CAP-Gly domain structure and uses thereof

PUBLICATION-DATE: November 13, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Luo, Ming	Vestavia Hills	AL	US

US-CL-CURRENT: 435/7.1; 530/350, 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

☐ 73. Document ID: US 20030203467 A1

L9: Entry 73 of 101 File: PGPB Oct 30, 2003

PGPUB-DOCUMENT-NUMBER: 20030203467
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20030203467 A1

TITLE: Novel variant EGIII-like cellulase compositions

PUBLICATION-DATE: October 30, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Gualfetti, Peter	San Francisco	CA	US
Mitchinson, Colin	Half Moon Bay	CA	US
Phillips, Jay	Palo Alto	CA	US

US-CL-CURRENT: 435/209; 435/105, 435/254.3, 435/320.1, 435/69.1, 510/320, 536/23.2

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

☐ 74. Document ID: US 20030199071 A1

L9: Entry 74 of 101 File: PGPB Oct 23, 2003

PGPUB-DOCUMENT-NUMBER: 20030199071
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20030199071 A1

TITLE: Mutant proteins, high potency inhibitory antibodies and fimch crystal structure

PUBLICATION-DATE: October 23, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Langermann, Solomon	Baltimore	MD	US
Hultgren, Scott J.	Town and Country	MO	US
Hung, Chia-Suei	St. Louis	MO	US
Bouckaert, Julie	St. Louis	MO	US

US-CL-CURRENT: 435/200; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

☐ 75. Document ID: US 20030198992 A1

L9: Entry 75 of 101 File: PGPB Oct 23, 2003

PGPUB-DOCUMENT-NUMBER: 20030198992
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20030198992 A1

TITLE: Treatment or prophylaxis of diseases caused by pilus-forming bacteria

PUBLICATION-DATE: October 23, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Hultgren, Scott	Ballwin	MO	US
Kuehn, Meta	Berkeley	CA	US
Xu, Zheng	Blue Bell	PA	US
Ogg, Derek	Stockholm	MO	SE
Harris, Mark	Uppsala		SE
Lepisto, Matti	Lund		SE
Jones, Charles Hal	Saint Louis		US
Kihlberg, Jan	Dalby		SE

US-CL-CURRENT: 435/7.1

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

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☐ 76. Document ID: US 20030186418 A1

L9: Entry 76 of 101 File: PGPB Oct 2, 2003

PGPUB-DOCUMENT-NUMBER: 20030186418
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20030186418 A1

TITLE: Novel variant EGIII-like cellulase compositions

PUBLICATION-DATE: October 2, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Gualfetti, Peter	San Francisco	CA	US
Mitchinson, Colin	Half Moon Bay	CA	US
Phillips, Jay	Palo Alto	CA	US

US-CL-CURRENT: 435/209; 435/101, 435/254.3, 435/320.1, 435/69.1, 536/23.2

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

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☐ 77. Document ID: US 20030175800 A1

L9: Entry 77 of 101 File: PGPB Sep 18, 2003

PGPUB-DOCUMENT-NUMBER: 20030175800
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20030175800 A1

TITLE: D1-C-terminal processing protease: methods for three dimensional structural determination and rational inhibitor design

PUBLICATION-DATE: September 18, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Diner, Bruce A.	Chadds Ford	PA	US
Jordan, Doug B.	Wilmington	DE	US
Liao, Der-Ing	Newark	DE	US
Nelson, Mark J.	Newark	DE	US

US-CL-CURRENT: 435/7.1; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

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☐ 78. Document ID: US 20030171327 A1

L9: Entry 78 of 101 File: PGPB Sep 11, 2003

PGPUB-DOCUMENT-NUMBER: 20030171327
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20030171327 A1

TITLE: Determination and uses of the atomic structures of ribosomes and ribosomal subunits and their ligand complexes

PUBLICATION-DATE: September 11, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Steitz, Thomas A.	Branford	CT	US
Moore, Peter B.	North Haven	CT	US
Ban, Nenad	Zurich	CT	CH
Nissen, Poul	Aarhus N		DK
Hansen, Jeffrey	New Haven		US

US-CL-CURRENT: 514/44; 536/23.1, 702/20

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

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☐ 79. Document ID: US 20030153002 A1

L9: Entry 79 of 101 File: PGPB Aug 14, 2003

PGPUB-DOCUMENT-NUMBER: 20030153002

PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20030153002 A1

TITLE: Ribosome structure and protein synthesis inhibitors

PUBLICATION-DATE: August 14, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Steitz, Thomas A.	Branford	CT	US
Moore, Peter B.	North Haven	CT	US
Ban, Nenad	New Haven	CT	US
Nissen, Poul	Aarhus N	CT	DK
Hansen, Jeffrey	New Haven	CT	US
Ippolito, Joseph A.	Guilford		US

US-CL-CURRENT: 435/7.1; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw D

☐ 80. Document ID: US 20030143714 A1

L9: Entry 80 of 101 File: PGPB Jul 31, 2003

PGPUB-DOCUMENT-NUMBER: 20030143714
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20030143714 A1

TITLE: Crystal structure of a mutant of cathepsin S enzyme

PUBLICATION-DATE: July 31, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Lamers, Marieke B.A.C.	Cambridge		GB
Williams, David H.	Cambridge		GB
Turkenburg, Johan P.	York		GB
Hubbard, Roderick E.	York		GB

US-CL-CURRENT: 435/226; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw D

☐ 81. Document ID: US 20030105326 A1

L9: Entry 81 of 101 File: PGPB Jun 5, 2003

PGPUB-DOCUMENT-NUMBER: 20030105326
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20030105326 A1

TITLE: Alkaloid halide salts of swainsonine and methods of use

PUBLICATION-DATE: June 5, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Dennis, James W.	Etobicoke		CA
Shah, Rajan N.	Toronto		CA
Ziser, Lothar	Toronto		CA

US-CL-CURRENT: 546/121

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

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☐ 82. Document ID: US 20030099955 A1

L9: Entry 82 of 101 File: PGPB May 29, 2003

PGPUB-DOCUMENT-NUMBER: 20030099955
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20030099955 A1

TITLE: Crystal structure of ribosomal protein L11/GTPase activating region rRNA and uses thereof

PUBLICATION-DATE: May 29, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Wimberly, Brian T.	Guilford	CT	US
Ramakrishnan, Venkatraman	Salt Lake City	UT	US

US-CL-CURRENT: 435/6; 435/199, 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

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☐ 83. Document ID: US 20030092645 A1

L9: Entry 83 of 101 File: PGPB May 15, 2003

PGPUB-DOCUMENT-NUMBER: 20030092645
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20030092645 A1

TITLE: PERIPHERAL NERVOUS SYSTEM SPECIFIC SODIUM CHANNELS, DNA ENCODING THEREFOR CRYSTALLIZATION, X-RAY DIFFRACTION, COMPUTER MOLECULAR MODELING, RATIONAL DRUG DESIGN, DRUG SCREENING, AND METHODS OF MAKING AND USING THEREOF

PUBLICATION-DATE: May 15, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
MANDEL, GAIL	STONY BROOK	NY	US
HALEGOUA, SIMON	BELLE TERRE	NY	US

US-CL-CURRENT: 514/44; 435/69.1

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

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☐ 84. Document ID: US 20030082622 A1

L9: Entry 84 of 101 File: PGPB May 1, 2003

PGPUB-DOCUMENT-NUMBER: 20030082622
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20030082622 A1

TITLE: Method of identifying inhibitors of Tie-2

PUBLICATION-DATE: May 1, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Bump, Nancy J.	Lowell	MA	US
Arnold, Lee D.	Westborough	MA	US
Dixon, Richard W.	Jefferson	MA	US
Heoffken, Hans Wolfgang	Ludwigshafen	MA	DE
Allen, Karen	Weston	CA	US
Bellamacina, Cornelia	Castro Valley		US

US-CL-CURRENT: 435/7.1; 530/350, 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

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☐ 85. Document ID: US 20030068831 A1

L9: Entry 85 of 101 File: PGPB Apr 10, 2003

PGPUB-DOCUMENT-NUMBER: 20030068831
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20030068831 A1

TITLE: Proteins and druggable regions of proteins

PUBLICATION-DATE: April 10, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Edwards, Aled	Toronto	CA	CA
Arrowsmith, Cheryl	North York		CA

Greenblatt, Jack	Toronto	CA
Mendlein, John D.	Encincitas	US

US-CL-CURRENT: 436/518; 435/7.1, 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw D

☐ 86. Document ID: US 20030068651 A1

L9: Entry 86 of 101 File: PGPB Apr 10, 2003

PGPUB-DOCUMENT-NUMBER: 20030068651
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20030068651 A1

TITLE: Multi-target analysis of gene families for chemistry of high affinity and selective small molecules and other therapeutics

PUBLICATION-DATE: April 10, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Arrowsmith, Cheryl	North York	CA	CA
Greenblatt, Jack	Toronto		CA
Edwards, Aled	Toronto		CA
Mendlein, John D.	Encincitas		US

US-CL-CURRENT: 435/7.1; 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw D

☐ 87. Document ID: US 20030068650 A1

L9: Entry 87 of 101 File: PGPB Apr 10, 2003

PGPUB-DOCUMENT-NUMBER: 20030068650
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20030068650 A1

TITLE: Target analysis for chemistry of specific and broad spectrum anti-infectives and other therapeutics

PUBLICATION-DATE: April 10, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Greenblatt, Jack	Toronto	CA	CA
Edwards, Aled	Toronto		CA
Arrowsmith, Cheryl	North York		CA
Mendlein, John D.	Encincitas		US

US-CL-CURRENT: 435/7.1; 435/5

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

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☐ 88. Document ID: US 20030036529 A1

L9: Entry 88 of 101 File: PGPB Feb 20, 2003

PGPUB-DOCUMENT-NUMBER: 20030036529
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20030036529 A1

TITLE: Compositions and methods for inhibiting arginase activity

PUBLICATION-DATE: February 20, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Christianson, David	Media	PA	US
Baggio, Ricky	Waltham	MA	US
Elbaum, Daniel	Newton	MA	US

US-CL-CURRENT: 514/64; 562/7

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

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☐ 89. Document ID: US 20020197628 A1

L9: Entry 89 of 101 File: PGPB Dec 26, 2002

PGPUB-DOCUMENT-NUMBER: 20020197628
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20020197628 A1

TITLE: Screening methods for identifying ligands

PUBLICATION-DATE: December 26, 2002

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Stewart, Lansing J.	Bainbridge Island	WA	US

US-CL-CURRENT: 435/6; 435/7.1, 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

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☐ 90. Document ID: US 20020187512 A1

L9: Entry 90 of 101 File: PGPB Dec 12, 2002

PGPUB-DOCUMENT-NUMBER: 20020187512
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20020187512 A1

TITLE: Crystal structure of human interleukin-22

PUBLICATION-DATE: December 12, 2002

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Nagem, Ronaldo Alves Pinto	Campinas	NY	BR
Polikarpov, Igor	Sao Carlos	NY	BR
Renauld, Jean Christophe	New York	NY	US
Colau, Didier	New York		US
Dumoutier, Laure	New York		US

US-CL-CURRENT: 435/7.1; 435/69.52, 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw De

Clear | Generate Collection | Print | Fwd Refs | Bkwd Refs | Generate OACS

Terms	Documents
L8 and reflection	101

Display Format: CIT Change Format

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Hit List

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Search Results - Record(s) 91 through 101 of 101 returned.

☐ 91. Document ID: US 20020183249 A1

L9: Entry 91 of 101 File: PGPB Dec 5, 2002

PGPUB-DOCUMENT-NUMBER: 20020183249
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20020183249 A1

TITLE: Method of identifying inhibitors of CDC25

PUBLICATION-DATE: December 5, 2002

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Taylor, Neil R.	Sydney	MA	AU
Borhani, David	Worcester	MA	US
Epstein, David	Belmont	NC	US
Rudolph, Johannes	Durham	MA	US
Ritter, Kurt	Newton	MA	US
Fujimori, Taro	Shrewsbury	MA	US
Robinson, Simon	Stow	MA	US
Eckstein, Jens	Arlington	CA	US
Haupt, Andreas	Schwetzingen	MA	DE
Walker, Nigel	Burlingame	MA	US
Dixon, Richard W.	Jefferson	MA	US
Choquette, Deborah	Rutland	MA	US
Blanchard, Jill	Arlington	MA	US
Kluge, Arthur	Lincoln	MA	US
Pal, Kollol	Needham	MA	US
Bockovich, Nicholas	Malden	MA	US
Come, Jon	Cambridge		US
Hediger, Mark	Marlboro		US

US-CL-CURRENT: 514/12; 435/226, 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

☐ 92. Document ID: US 20020146428 A1

L9: Entry 92 of 101 File: PGPB Oct 10, 2002

PGPUB-DOCUMENT-NUMBER: 20020146428
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20020146428 A1

TITLE: Treatment or prophylaxis of diseases caused by pilus-forming bacteria

PUBLICATION-DATE: October 10, 2002

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Hultgren, Scott	Ballwin	MO	US
Kuehn, Meta	Berkeley	CA	US
Xu, Zheng	Blue Bell	PA	US
Ogg, Derek	Stockholm	MO	SE
Harris, Mark	Uppsala		SE
Lepisto, Matti	Lund		SE
Jones, Charles Hal	Saint Louis		US
Kihlberg, Jan	Dalby		SE

US-CL-CURRENT: 424/190.1; 424/242.1, 435/183, 435/252.3

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

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☐ 93. Document ID: US 20020107359 A1

L9: Entry 93 of 101 File: PGPB Aug 8, 2002

PGPUB-DOCUMENT-NUMBER: 20020107359
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20020107359 A1

TITLE: THREE DIMENSIONAL STRUCTURES AND MODELS OF FC RECEPTORS AND USES THEREOF

PUBLICATION-DATE: August 8, 2002

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
HOGARTH, P. MARK	WILLIAMSTOWN		AU
POWELL, MAREE S.	FERNTREE GULLY		AU
MCKENZIE, IAN F.C.	BRUNSWICK		AU
MAXWELL, KELLY F.	SOUTH YARRA		AU
GARRETT, THOMAS P.J.	BRUNSWICK		AU
EPA, VIDANA	PARKVILLE		AU

US-CL-CURRENT: 530/350; 436/86, 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

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☐ 94. Document ID: US 20020086308 A1

L9: Entry 94 of 101 File: PGPB Jul 4, 2002

PGPUB-DOCUMENT-NUMBER: 20020086308
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20020086308 A1

TITLE: Ribosome structure and protein synthesis inhibitors

PUBLICATION-DATE: July 4, 2002

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Steitz, Thomas A.	Branford	CT	US
Moore, Peter B.	New Haven	CT	US
Ban, Nenad	Riedenhalden	CT	CH
Nissen, Poul	Aarhus N		DK
Hansen, Jeffrey	New Haven		US

US-CL-CURRENT: 435/6; 378/73, 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw D

☐ 95. Document ID: US 20020061539 A1

L9: Entry 95 of 101 File: PGPB May 23, 2002

PGPUB-DOCUMENT-NUMBER: 20020061539
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20020061539 A1

TITLE: METHODS AND COMPOUNDS FOR MODULATING NUCLEAR RECEPTOR COACTIVATOR BINDING

PUBLICATION-DATE: May 23, 2002

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
BAXTER, JOHN D.	SAN FRANCISCO	CA	US
DARIMONT, BEATRICE	SAN FRANCISCO	CA	US
FENG, WEIJUN	SAN FRANCISCO	CA	US
FLETTERICK, ROBERT J.	SAN FRANCISCO	CA	US
KUSHNER, PETER J.	SAN FRANCISCO	CA	US
WAGNER, RICHARD L.	SAN FRANCISCO	CA	US
WEST, BRIAN L.	SAN FRANCISCO	CA	US
YAMAMOTO, KEITH R.	SAN FRANCISCO	CA	US

US-CL-CURRENT: 435/7.1; 257/E21.218, 257/E21.266, 435/183, 435/4, 702/19, 702/27

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWMC | Draw D

☐ 96. Document ID: US 20020045599 A1

L9: Entry 96 of 101 File: PGPB Apr 18, 2002

PGPUB-DOCUMENT-NUMBER: 20020045599
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20020045599 A1

TITLE: Nucleotide analog compositions

PUBLICATION-DATE: April 18, 2002

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Arimilli, Murty N.	Fremont	CA	US
Kelly, Daphne E.	San Francisco	CA	US
Lee, Thomas T.K.	Redwood City	CA	US
Manes, Lawrence V.	Moss Beach	CA	US
Munger, John D. JR.	Alviso	CA	US
Prisbe, Ernest J.	Los Altos	CA	US
Schultze, Lisa M.	San Carlos	CA	US

US-CL-CURRENT: 514/81; 544/244

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw De

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☐ 97. Document ID: US 20020045199 A1

L9: Entry 97 of 101 File: PGPB Apr 18, 2002

PGPUB-DOCUMENT-NUMBER: 20020045199
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20020045199 A1

TITLE: Treatment or prophylaxis of diseases caused by pilus-forming bacteria

PUBLICATION-DATE: April 18, 2002

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Hultgren, Scott	Ballwin	MO	US
Kuehn, Meta	Berkeley	CA	US
Xu, Zheng	Blue Bell	PA	US
Ogg, Derek	Stockholm	MO	SE
Harris, Mark	Uppsala		SE
Lepisto, Matti	Lund		SE
Jones, Charles Hal	Saint Louis		US
Kihlberg, Jan	Dalby		SE

US-CL-CURRENT: 435/7.32; 514/23, 536/116, 546/242, 549/28

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw D

☐ 98. Document ID: US 20020034774 A1

L9: Entry 98 of 101 File: PGPB Mar 21, 2002

PGPUB-DOCUMENT-NUMBER: 20020034774
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20020034774 A1

TITLE: Treatment or prophylaxis of diseases caused by pilus-forming bacteria

PUBLICATION-DATE: March 21, 2002

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Hultgren, Scott	Ballwin	MO	US
Kuehn, Meta	Berkeley	CA	US
Xu, Zheng	Blue Bell	PA	US
Ogg, Derek	Stockholm	MO	SE
Harris, Mark	Uppsala		SE
Lepisto, Matti	Lund		SE
Jones, Charles Hal	Saint Louis		US
Kihlberg, Jan	Dalby		SE

US-CL-CURRENT: 435/7.32; 536/116, 536/117, 536/4.1, 536/53

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw D

☐ 99. Document ID: US 20020031782 A1

L9: Entry 99 of 101 File: PGPB Mar 14, 2002

PGPUB-DOCUMENT-NUMBER: 20020031782
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20020031782 A1

TITLE: Mycobacterium tuberculosis CYP51 high resolution structure, polypeptides and nucleic acids, and therapeutic and screening methods relating to same

PUBLICATION-DATE: March 14, 2002

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Waterman, Michael R.	Nashville	TN	US
Bellamine, Aouatef	Nashville	TN	US
Podust, Larissa M.	Hermitage	TN	US

US-CL-CURRENT: 435/7.1; 435/183, 702/19

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

☐ 100. Document ID: US 20020012979 A1

L9: Entry 100 of 101 File: PGPB Jan 31, 2002

PGPUB-DOCUMENT-NUMBER: 20020012979
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20020012979 A1

TITLE: VITAMIN C PRODUCTION IN MICROORGANISMS AND PLANTS

PUBLICATION-DATE: January 31, 2002

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
BERRY, ALAN	BLOOMFIELD	NJ	US
RUNNING, JEFFREY A.	MANITOWOC	WI	US
SEVERSON, DAVID K.	TWO RIVERS	WI	US
BURLINGGAME, RICHARD P.	MANITOWOC	WI	US

US-CL-CURRENT: 435/136; 435/233, 435/243, 435/252.3, 435/252.31, 435/252.32, 435/252.33, 435/252.34, 435/252.35, 435/254.1, 435/254.11, 435/254.21

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

☐ 101. Document ID: US 20010039479 A1

L9: Entry 101 of 101 File: PGPB Nov 8, 2001

PGPUB-DOCUMENT-NUMBER: 20010039479
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20010039479 A1

TITLE: Three-dimensional model of a Fc region of an IgE antibody and uses thereof

PUBLICATION-DATE: November 8, 2001

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY
Jardetzky, Theodore S.	Chicago	IL	US
Wurzburg, Beth A.	Evanston	IL	US

US-CL-CURRENT: 702/19; 530/388.1

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. De

Clear | Generate Collection | Print | Fwd Refs | Bkwd Refs | Generate OACS

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FILE 'HOME' ENTERED AT 11:37:39 ON 26 JAN 2006

=> file reg
=> s e64/cn
'E64' NOT FOUND
The E# entered is not currently defined.

=> s (e64)/cn
'E64' NOT FOUND
The E# entered is not currently defined.

=> s (e64)
'E64' NOT FOUND
The E# entered is not currently defined.

=> file .nash
=> s (cathepsin or Scats) and crystal? and x-ray
L1          131 FILE MEDLINE
L2          103 FILE CAPLUS
L3          119 FILE SCISEARCH
L4           11 FILE LIFESCI
L5           59 FILE BIOSIS
L6           79 FILE EMBASE

TOTAL FOR ALL FILES
L7          502 (CATHEPSIN OR SCATS) AND CRYSTAL? AND X-RAY

=> s l7 and human
TOTAL FOR ALL FILES
L14         291 L7 AND HUMAN

=> s e64
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=> s (e64)
'E64' NOT FOUND
The E# entered is not currently defined.

=> s l14 and e64
'E64' NOT FOUND
The E# entered is not currently defined.

=> s l14 and (ligand or complex?)
TOTAL FOR ALL FILES
L21         129 L14 AND (LIGAND OR COMPLEX?)

=> dup rem l21
PROCESSING COMPLETED FOR L21
L22          79 DUP REM L21 (50 DUPLICATES REMOVED)

=> s l21 not 2004-2006/py
TOTAL FOR ALL FILES
L29         108 L21 NOT 2004-2006/PY

=> dup rem l29
PROCESSING COMPLETED FOR L29
L30          63 DUP REM L29 (45 DUPLICATES REMOVED)

=> d ibib abs 1-63

L30  ANSWER 1 OF 63  CAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:        2003:590728  CAPLUS Full-text
DOCUMENT NUMBER:         139:145839
TITLE:                   Crystal structure of a human
                         cathepsin S mutant, apparatus displaying a
                         three-dimensional representation of the
                         cathepsin S and applications to drug screening
                         and design
INVENTOR(S):             Lamers, Marieke B.; Williams, David H.; Turkenburg,
```

Johan P.; Hubbard, Roderick E.
PATENT ASSIGNEE(S): Medivir Uk Ltd., UK
SOURCE: U.S. Pat. Appl. Publ., 59 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003143714	A1	20030731	US 2002-273577	20021018
PRIORITY APPLN. INFO.:			US 2001-330191P P	20011019

AB The invention relates to the X-ray crystal structure of a human cathepsin S mutant. The invention further relates to an apparatus programmed with one or more of the structure coordinates of the cathepsin S binding pockets, wherein said apparatus is capable of displaying a three-dimensional representation of that binding pocket. The invention also relates to methods of using the structure coordinates of a mutant cathepsin S to screen and design compds. that bind to the active site and accessory binding site of cathepsin S.

L30 ANSWER 2 OF 63 MEDLINE on STN DUPLICATE 1
ACCESSION NUMBER: 2003608123 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 14690410
TITLE: Peptide ketobenzoxazole inhibitors bound to cathepsin K.
AUTHOR: McGrath Mary E; Sprengeler Paul A; Hill Craig M; Martichonok Valeri; Cheung Harry; Somoza John R; Palmer James T; Janc James W
CORPORATE SOURCE: Celera, South San Francisco, California 94080, USA.. mary.mcgrath@celera.com
SOURCE: Biochemistry, (2003 Dec 30) 42 (51) 15018-28.
Journal code: 0370623. ISSN: 0006-2960.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200405
ENTRY DATE: Entered STN: 20031224
Last Updated on STN: 20040505
Entered Medline: 20040504

AB Potent inhibitors of human cysteine proteases of the papain family have been made and assayed versus a number of relevant family members. We describe the synthesis of peptide alpha-ketoheterocyclic inhibitors that occupy binding subsites S1'-S3 of the cysteine protease substrate recognition cleft and that form a reversible covalent bond with the Cys 25 nucleophile. X-ray crystal structures of cathepsin K both unbound and complexed with inhibitors provide detailed information on protease/inhibitor interactions and suggestions for the design of tight-binding, selective molecules.

L30 ANSWER 3 OF 63 MEDLINE on STN
ACCESSION NUMBER: 2003143398 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 12641451
TITLE: Specificity determinants of human cathepsin s revealed by crystal structures of complexes.
AUTHOR: Pauly Thomas A; Sulea Traian; Ammirati Mark; Sivaraman J; Danley Dennis E; Griffor Matthew C; Kamath Ajith V; Wang I-K; Laird Ellen R; Seddon Andrew P; Menard Robert; Cygler Miroslaw; Rath Virginia L
CORPORATE SOURCE: Exploratory Medicinal Sciences and Computational Chemistry, Groton Laboratories, Pfizer Global Research and Development, Eastern Point Road, Groton, Connecticut 06340, USA.
SOURCE: Biochemistry, (2003 Mar 25) 42 (11) 3203-13.
Journal code: 0370623. ISSN: 0006-2960.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
OTHER SOURCE: PDB-1NPZ; PDB-1NQC

ENTRY MONTH: 200304
ENTRY DATE: Entered STN: 20030328
Last Updated on STN: 20030418
Entered Medline: 20030417

AB Cathepsin S, a lysosomal cysteine protease of the papain superfamily, has been implicated in the preparation of MHC class II alphabeta-heterodimers for antigen presentation to CD4+ T lymphocytes and is considered a potential target for autoimmune-disease therapy. Selective inhibition of this enzyme may be therapeutically useful for attenuating the hyperimmune responses in a number of disorders. We determined the three-dimensional crystal structures of human cathepsin S in complex with potent covalent inhibitors, the aldehyde inhibitor 4-morpholinecarbonyl-Phe-(S- benzyl)Cys-Psi(CH=O), and the vinyl sulfone irreversible inhibitor 4-morpholinecarbonyl-Leu-Hph-Psi(CH=CH-SO(2)-phenyl) at resolutions of 1.8 and 2.0 A, respectively. In the structure of the cathepsin S-aldehyde complex, the tetrahedral thiohemiacetal adduct favors the S-configuration, in which the oxygen atom interacts with the imidazole group of the active site His164 rather than with the oxyanion hole. The present structures provide a detailed map of noncovalent intermolecular interactions established in the substrate-binding subsites S3 to S1' of cathepsin S. In the S2 pocket, which is the binding affinity hot spot of cathepsin S, the Phe211 side chain can assume two stable conformations that accommodate either the P2-Leu or a bulkier P2-Phe side chain. This structural plasticity of the S2 pocket in cathepsin S explains the selective inhibition of cathepsin S over cathepsin K afforded by inhibitors with the P2-Phe side chain. Comparison with the structures of cathepsins K, V, and L allows delineation of local intermolecular contacts that are unique to cathepsin S.

L30 ANSWER 4 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 2003:575478 CAPLUS Full-text
DOCUMENT NUMBER: 140:37836
TITLE: A new class of inhibitors for the malarial aspartic protease plasmepsin II based on a central 11-azatricyclo[6.2.1.02,7]undeca-2,4,6-triene scaffold
AUTHOR(S): Carcache, David A.; Hoertner, Simone R.; Bertogg, Andreas; Diederich, Francois; Dorn, Arnulf; Maerki, Hans Peter; Binkért, Christoph; Bur, Daniel
CORPORATE SOURCE: Laboratorium fuer Organische Chemie der Eidgenoessischen Technischen Hochschule, ETH-Hoenggerberg, HCI, Zurich, CH-8093, Switz.
SOURCE: Helvetica Chimica Acta (2003), 86(6), 2192-2209
CODEN: HCACAV; ISSN: 0018-019X
PUBLISHER: Verlag Helvetica Chimica Acta
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A new class of nonpeptidic inhibitors of the malarial aspartic protease plasmepsin II (PMII) with up to single-digit micromolar activities (IC50 values) was developed by structure-based de novo design. The active-site matrix used in the design was based on an x-ray crystal structure of PMII, onto which the major conformational changes seen in the structure of renin upon complexation of 4-arylpiperidines-including the unlocking of a new hydrophobic (flap) pocket - were modeled. The sequence identity of 35% between mature renin and PMII had prompted us to hypothesize that an induced-fit adaptation around the active site as observed in renin might also be effective in PMII. The new inhibitors contain a central 11-azatricyclo[6.2.1.02,7]undeca- 2(7),3,5-triene core, which, in protonated form, undergoes ionic H-bonding with the two catalytic Asp residues at the active site of PMII (Figs. 1 and 2). This tricyclic scaffold is readily prepared by a Diels-Alder reaction between an activated pyrrole and a benzyne species generated in situ (Scheme 1). Two substituents with naphthyl or 1,3-benzothiazole moieties are attached to the central core (Schemes 1-4) for accommodation in the hydrophobic flap and S1/S3 (or S2', depending on the optical antipode of the inhibitor) pockets at the active site of the enzyme. The most potent inhibitors (±)-19a-19c (1C50 3-5 μM) and (±)-23b (2 μM) (Table) bear an addnl. Cl-atom on the 1,3-benzothiazole moiety to fully fill the rear of the flap pocket. Optimization of the linker between the tricyclic scaffold and the 1,3-benzothiazole moiety, based on detailed conformational anal. (Figs. 3 and 4), led to a further small increase in inhibitory strength. The new compds. were also tested against other aspartic proteases. They were found to be quite selective against renin, while the selectivity against cathepsin D and E, two other human aspartic proteases, is rather poor (Table). The detailed SARs established in this investigation provide a valuable basis for the design of the next generations of more-potent and -selective PMII inhibitors with potential application in a new antimalarial therapy.

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 5 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:661389 CAPLUS Full-text
DOCUMENT NUMBER: 140:104196
TITLE: Design of β-lactams with mechanism based nonantibacterial activities
AUTHOR(S): Veinberg, Grigory; Vorona, Maxim; Shestakova, Irina; Kanepe, Iveta; Lukevics, Edmunds
CORPORATE SOURCE: Latvian Institute of Organic Synthesis, Riga, LV 1006, Latvia
SOURCE: Current Medicinal Chemistry (2003), 10(17), 1741-1757
CODEN: CMCHE7; ISSN: 0929-8673
PUBLISHER: Bentham Science Publishers Ltd.
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review. The majority of nonantibacterial activities discovered for β-lactam derivs. during the last 15 yr are based on their ability to form a stable covalent complex with nucleophile in the active site of enzymes regulating fundamental physiol. processes in mammalian organism such as serine and cysteine proteases, LDL phospholipase A2, A-independent transacylase and some still indeciphered enzymes. Regulation of their catalytic activity both in vitro and in vivo by compds. designed on the cephalosporin, penicillin and 2-azetidinone base was successfully exploited in the treatment of inflammatory, respiratory, cardiovascular disorders, cancer and other pathol. processes. Availability of x-ray crystallog. data for target enzymes and computational mol. modeling in combination with wide possibilities of structural modifications for com. natural and synthetic β-lactams and the chiral blocks allow to consider this class of organic compds. as a perspective source of mechanism based nonantibacterial drugs.

REFERENCE COUNT: 72 THERE ARE 72 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 6 OF 63 MEDLINE on STN
ACCESSION NUMBER: 2003071876 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 12581647
TITLE: Crystal structure of Stefin A in complex with cathepsin H: N-terminal residues of inhibitors can adapt to the active sites of endo- and exopeptidases.
AUTHOR: Jenko Sasa; Dolenc Iztok; Guncar Gregor; Dobersek Andreja; Podobnik Marjetka; Turk Dusan
CORPORATE SOURCE: Department of Biochemistry and Molecular Biology, Jozef Stefan Institute, Jamova 39, SI-1111 Ljubljana, Slovenia.
SOURCE: Journal of molecular biology, (2003 Feb 21) 326 (3) 875-85.
Journal code: 2985088R. ISSN: 0022-2836.
PUB. COUNTRY: England: United Kingdom
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
OTHER SOURCE: PDB-1NB3; PDB-1NB5
ENTRY MONTH: 200303
ENTRY DATE: Entered STN: 20030214
Last Updated on STN: 20030314
Entered Medline: 20030313

AB Binding of cystatin-type inhibitors to papain-like exopeptidases cannot be explained by the stefin B-papain complex. The crystal structure of human stefin A bound to an aminopeptidase, porcine cathepsin H, has been determined in monoclinic and orthorhombic crystal forms at 2.8A and 2.4A resolutions, respectively. The asymmetric unit of each form contains four complexes. The structures are similar to the stefin B-papain complex, but with a few distinct differences. On binding, the N-terminal residues of stefin A adopt the form of a hook, which pushes away cathepsin H mini-chain residues and distorts the structure of the short four residue insertion (Lys155A-Asp155D) unique to cathepsin H. Comparison with the structure of isolated cathepsin H shows that the rims of the cathepsin H structure are slightly displaced (up to 1A) from their position in the free enzyme. Furthermore, comparison with the stefin B-papain complex showed that molecules of stefin A bind about 0.8A deeper into the active site cleft of cathepsin H than stefin B into papain. The approach of stefin A to cathepsin H induces structural changes along the interaction surface of both molecules, whereas no such changes were observed in the stefin B-papain complex. Carboxymethylation of papain seems to have prevented the formation of the genuine binding geometry between a papain-like enzyme and a cystatin-type inhibitor as we observe it in the structure presented here.

L30 ANSWER 7 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:937303 CAPLUS Full-text

DOCUMENT NUMBER: 138:20443
TITLE: Endocrine disruptor screening using DNA chips of endocrine disruptor-responsive genes
INVENTOR(S): Kondo, Akihiro; Takeda, Takeshi; Mizutani, Shigetoshi; Tsujimoto, Yoshimasa; Takashima, Ryokichi; Enoki, Yuki; Kato, Ikunoshin
PATENT ASSIGNEE(S): Takara Bio Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 386 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
JP 2002355079	A2	20021210	JP 2002-69354		20020313
PRIORITY APPLN. INFO.:			JP 2001-73183	A	20010314
			JP 2001-74993	A	20010315
			JP 2001-102519	A	20010330

AB A method and kit for detecting endocrine-disrupting chems. using DNA microarrays are claimed. The method comprises preparing a nucleic acid sample containing mRNAs or cDNAs originating in cells, tissues, or organisms which have been brought into contact with a sample containing the endocrine disruptor. The nucleic acid sample is hybridized with DNA microarrays having genes affected by the endocrine disruptor or DNA fragments originating in these genes have been fixed. The results obtained are then compared with the results obtained with the control sample to select the gene affected by the endocrine disruptor. Genes whose expression is altered by tri-Bu tin, 4-octaphenol, 4-nonylphenol, di-N-Bu phthalate, dichlorohexyl phthalate, octachlorostyrene, benzophenone, diethylhexyl phthalate, diethylstilbestrol (DES), and 17-β estradiol (E2), were found in mice by DNA chip anal.

L30 ANSWER 8 OF 63 MEDLINE on STN
ACCESSION NUMBER: 2002663671 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 12423365
TITLE: The role of the second binding loop of the cysteine protease inhibitor, cystatin A (stefin A), in stabilizing complexes with target proteases is exerted predominantly by Leu73.
AUTHOR: Pavlova Alona; Bjork Ingemar
CORPORATE SOURCE: Department of Veterinary Medical Chemistry, Swedish University of Agricultural Sciences, Uppsala Biomedical Centre, Sweden.
SOURCE: European journal of biochemistry / FEBS, (2002 Nov) 269 (22) 5649-58.
Journal code: 0107600. ISSN: 0014-2956.
PUB. COUNTRY: Germany: Germany, Federal Republic of
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200301
ENTRY DATE: Entered STN: 20021109
Last Updated on STN: 20030115
Entered Medline: 20030114

AB The aim of this work was to elucidate the roles of individual residues within the flexible second binding loop of human cystatin A in the inhibition of cysteine proteases. Four recombinant variants of the inhibitor, each with a single mutation, L73G, P74G, Q76G or N77G, in the most exposed part of this loop were generated by PCR-based site-directed mutagenesis. The binding of these variants to papain, cathepsin L, and cathepsin B was characterized by equilibrium and kinetic methods. Mutation of Leu73 decreased the affinity for papain, cathepsin L and cathepsin B by approximately 300-fold, >10-fold and approximately 4000-fold, respectively. Mutation of Pro74 decreased the affinity for cathepsin B by approximately 10-fold but minimally affected the affinity for the other two enzymes. Mutation of Gln76 and Asn77 did not alter the affinity of cystatin A for any of the proteases studied. The decreased affinities were caused exclusively by increased dissociation rate constants. These results show that the second binding loop of cystatin A plays a major role in stabilizing the complexes with proteases by retarding their dissociation. In contrast with cystatin B, only one amino-acid residue of the loop, Leu73, is of principal importance for this effect, Pro74 assisting to a minor extent only in the case of cathepsin B binding. The contribution of the second binding loop of

cystatin A to protease binding varies with the protease, being largest, approximately 45% of the total binding energy, for inhibition of cathepsin B.

L30 ANSWER 9 OF 63 MEDLINE on STN DUPLICATE 3
ACCESSION NUMBER: 2002671360 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 12431059
TITLE: Design of noncovalent inhibitors of human cathepsin L. From the 96-residue proregion to optimized tripeptides.
AUTHOR: Chowdhury Shafinaz F; Sivaraman J; Wang Jing; Devanathan Gopal; Lachance Paule; Qi Hongtao; Menard Robert; Lefebvre Jean; Konishi Yasuo; Cygler Miroslaw; Sulea Traian; Purisima Enrico O
CORPORATE SOURCE: Biotechnology Research Institute, National Research Council of Canada, 6100 Royalmount Avenue, Montreal, Quebec, H4P 2R2, Canada.
SOURCE: Journal of medicinal chemistry, (2002 Nov 21) 45 (24) 5321-9.
Journal code: 9716531. ISSN: 0022-2623.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
OTHER SOURCE: PDB-1MHW
ENTRY MONTH: 200212
ENTRY DATE: Entered STN: 20021115
Last Updated on STN: 20021221
Entered Medline: 20021220

AB A novel series of noncovalent inhibitors of cathepsin L have been designed to mimic the mode of autoinhibition of procathepsin L. Just like the propeptide, these peptide-based inhibitors have a reverse-binding mode relative to a substrate and span both the S' and S subsites of the enzyme active site. In contrast to previous studies in which even moderate truncation of the full-length propeptide led to rapid reduction in potency, these blocked tripeptide-sized inhibitors maintain nanomolar potency. Moreover, these short peptides show higher selectivity (up to 310-fold) for inhibiting cathepsin L over K versus only 2-fold selectivity of the 96-residue propeptide of cathepsin L. A 1.9 A X-ray crystallographic structure of the complex of cathepsin L with one of the inhibitors confirms the designed reverse-binding mode of the inhibitor as well as its noncovalent nature. Enzymatic analysis also shows the inhibitors to be resistant to hydrolysis at elevated concentrations of the enzyme. The mode of inhibition of these molecules provides a general strategy for inhibiting other cathepsins as well as other proteases.

L30 ANSWER 10 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:207068 CAPLUS Full-text
DOCUMENT NUMBER: 136:395323
TITLE: Nonpeptide Inhibitors of Cathepsin G: Optimization of a Novel β-Ketophosphonic Acid Lead by Structure-Based Drug Design
AUTHOR(S): Greco, Michael N.; Hawkins, Michael J.; Powell, Eugene T.; Almond, Harold R., Jr.; Corcoran, Thomas W.; de Garavilla, Lawrence; Kauffman, Jack A.; Recacha, Rosario; Chattopadhyay, Debashish; Andrade-Gordon, Patricia; Maryanoff, Bruce E.
CORPORATE SOURCE: Johnson Johnson Pharmaceutical Research & Development, Spring House, PA, 19477-0776, USA
SOURCE: Journal of the American Chemical Society (2002), 124(15), 3810-3811
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:395323

AB The serine protease cathepsin G (EC 3.4.21.20; Cat G), which is stored in the azurophilic granules of neutrophils (polymorphonuclear leukocytes) and released on degranulation, has been implicated in various pathol. conditions associated with inflammation. By employing high-throughput screening, we identified a β-ketophosphonic acid as a moderate inhibitor of Cat G (IC50 = 4.1 μM). We were fortunate to obtain a co-crystal of the same with Cat G and solve its structure by x-ray crystallog. (3.5 Å). Structural details from the x-ray anal. of the ligand bound Cat G served as a platform for optimization of this lead

compound by structure-based drug design. With the aid of mol. modeling, substituents were attached to the 3-position of the 2-naphthyl ring of the β-ketophosphonic acid, which occupies the S1 pocket of Cat G, to provide an extension into the hydrophobic S3 region. Thus, we arrived at an analog with an 80-fold potency improvement over the parent (IC50 = 53 nM). From these results, it is evident that the β-ketophosphonic acid unit can form the basis for a novel class of serine protease inhibitors.

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 11 OF 63 SCISEARCH COPYRIGHT (c) 2006 The Thomson Corporation on STN

ACCESSION NUMBER: 2003:126083 SCISEARCH Full-text
THE GENUINE ARTICLE: 637VM
TITLE: Coordination of deprotonated saccharin in copper(II) complexes. Structural role of the saccharinate directed by the ancillary N-heterocyclic ligands
AUTHOR: Naumov P (Reprint); Jovanovski G; Ristova M; Razak I A; Cakir S; Chantrapromma S; Fun H K; Ng S W
CORPORATE SOURCE: Tokyo Inst Technol, Dept Chem & Mat Sci, Ohashi Lab, Meguro Ku, Ookayama 2-12-1, Tokyo 1528551, Japan (Reprint); Sv Kiril & Metodij Univ, Inst Chem, Skopje, Macedonia; Univ Sains Malaysia, Sch Phys, Xray Crystallog, Penang, Madagascar; Ondokuz Mayis Univ, Fac Arts & Sci, Dept Chem, Samsun, Turkey; Prince Songkla Univ, Fac Sci, Dept Chem, Songkhla, Thailand; Univ Malaya, Inst Postgrad Studies, Kuala Lumpur, Malaysia
COUNTRY OF AUTHOR: Japan; Macedonia; Madagascar; Turkey; Thailand; Malaysia
SOURCE: ZEITSCHRIFT FUR ANORGANISCHE UND ALLGEMEINE CHEMIE, (DEC 2002) Vol. 628, No. 13, pp. 2930-2939.
ISSN: 0044-2313.
PUBLISHER: WILEY-V C H VERLAG GMBH, PO BOX 10 11 61, D-69451 WEINHEIM, GERMANY.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 65
ENTRY DATE: Entered STN: 14 Feb 2003
Last Updated on STN: 14 Feb 2003

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB Four different coordination patterns were observed following the partial or complete thermodynamically-controlled ligand substitution of the hydrated tetraaquabis(o-sulfobenzimidato-N)copper(II) complex with heterocyclic bases as examined by X- ray diffraction. The N-heterocycle directs the o-sulfobenzimidate (saccharinate) anion into the immediate coordination polyhedron of the metal by any of the imido, carbonyl or sulfonyl functionalities, or as a lattice counter-ion in the crystal lattice. Aqua(o-sulfobenzimidato-O)tetrakis(4-methylpyridine)copper(II) o-sulfobenzimidate hemihydrate (1) crystallizes in the monoclinic space group P2(1)/n [a = 14.7858(2), b = 16.9090(1), c = 26.2350(2)Angstrom; beta = 92.861(1)degrees], aquadi(o-sulfobenzimidato- N)bis(4-propylpyridine)copper(II) (2) in the tetragonal space group P4(2)/n [a = 15.4127(1), c = 13.4604(1) Angstrom], diaquatetrakis(3-(2- propenyl)imidazole)copper(II) di-o-sulfobenzimidate (3b) in the monoclinic space group P2(1)/c [a = 9.3959(5), b = 28.029(2), c = 8.8763(3) Angstrom; beta = 111.175(1)degrees] and di(o-sulfobenzimidato)tetra(isoquinoline)cop per(II) (4b) in the orthorhombic space group Pna2(1) [a = 23.2132(6), b = 11.5760(2), c = 17.6297(4) Angstrom]. The copper atom in 1 is six-coordinate in a distorted trans-N4O2Cu octahedron with elongated copper-oxygen bonds [Cu-O-water = 2.462(3), Cu-O-sulfonyl = 2.567(3) Angstrom]. This adduct represents the first example of a combined O-sulfonyl/ionic coordination of the o-sulfobenzimidate ion in the same crystal. The copper atom in 2 is five-coordinate in the form of a N4OCu square pyramid [Cu-O-water = 2.238(5) Angstrom]. In 3, the o-sulfobenzimidate anions are linked to the copper atom through the coordinated water molecule forming a distorted octahedral N4O2Cu environment. In 4, the copper atom is nearly octahedrally coordinated by four nitrogen atoms and a pair of o-sulfobenzimidate carbonyl oxygen atoms. The structural details of the o-sulfobenzimidate coordination pattern correspond well with the 298 and 77 K FT IR spectra of the adducts. The structures of two other solid adducts, tris(3-(2- propenyl)imidazole)copper(II) di-o-sulfobenzimidate trihydrate (3a) and diaquabis(o-sulfobenzimidato-N)bis(isoquinoline)copper(II) (4a) have been predicted by their spectral features. Alteration of the o-sulfobenzimidate coordination mode upon changing the heterocycle ligand shows that this moiety is as a convenient polyfunctional structural tool for the construction of functional solids.

L30 ANSWER 12 OF 63 EMBASE COPYRIGHT (c) 2006 Elsevier B.V. All rights reserved on STN

ACCESSION NUMBER: 2002412990 EMBASE Full-text
TITLE: Inhibitors of the protease domain of urokinase-type plasminogen activator.
AUTHOR: Rockway T.W.; Nienaber V.; Giranda V.L.
CORPORATE SOURCE: T.W. Rockway, Abbott Laboratories, 200 Abbott Park Road, Abbott Park, IL 60064-6217, United States. todd.w.rockway@abbott.com
SOURCE: Current Pharmaceutical Design, (2002) Vol. 8, No. 28, pp. 2541-2558.
Refs: 95
ISSN: 1381-6128 CODEN: CPDEFP
COUNTRY: Netherlands
DOCUMENT TYPE: Journal; General Review
FILE SEGMENT: 016 Cancer
030 Pharmacology
037 Drug Literature Index
LANGUAGE: English
SUMMARY LANGUAGE: English
ENTRY DATE: Entered STN: 20021202
Last Updated on STN: 20021202

AB Human urokinase-type plasminogen activator (uPA or uPA) has been implicated in the regulation and control of basement membrane and interstitial protein degradation. Since Urokinase plays a role in tissue remodeling, it may be responsible, in part, for the disease progression of cancer. Inhibitors of urokinase may then be useful in the treatment of cancer by retarding tumor growth and metastasis. Urokinase is a multidomain protein, two regions of the protein are most responsible for the observed proteolytic activity in cancer disease and progression. The N-terminal domain or ATF binds to a Urokinase receptor (uPAR) on the cell surface and the C-terminal serine protease domain, then, activates plasminogen to plasmin, beginning a cascade of events leading to the progression of cancer. Investigations of urokinase inhibition has been an area of ongoing research for the past 3 decades. It began with the discovery of small natural and unnatural amino acid derivatives or peptide analogs which exhibited weak inhibition of uPA. The last decade has seen the generation of several classes of potent and selective Urokinase inhibitor directed to the serine protease domain of the protein which have shown potential anti-cancer effects. The availability of structural information of enzyme-inhibitor complexes either by nuclear magnetic spectroscopy (NMR) or crystallography has allowed a detailed analysis of inhibitor protein interactions that contribute to observed inhibitor potency. Structural studies of specific inhibitor-uPA complexes will be discussed as well as the contributions of specific inhibitor protein interactions that are important for overall inhibitor potency. These data were used to discover a class of urokinase inhibitor based on the 2-Naphthamidine template that exhibits potent urokinase inhibition and excellent selectivity for urokinase over similar trypsin family serine proteases.

L30 ANSWER 13 OF 63 MEDLINE on STN DUPLICATE 4

ACCESSION NUMBER: 2002691822 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 12454497
TITLE: Expression, purification, crystallization and preliminary X-ray diffraction studies of human cathepsin F complexed with an irreversible vinyl sulfone inhibitor.
AUTHOR: Ho Joseph D; Meltser Yana; Buggy Joseph J; Palmer James T; Elrod Kyle C; Chan Hedy; Mortara Kyle D; Somoza John R
CORPORATE SOURCE: Celera Inc, 180 Kimball Way, South San Francisco, CA 94080, USA.
SOURCE: Acta crystallographica. Section D, Biological crystallography, (2002 Dec) 58 (Pt 12) 2187-90. Electronic Publication: 2002-11-23.
Journal code: 9305878. ISSN: 0907-4449.
PUB. COUNTRY: Denmark
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200306
ENTRY DATE: Entered STN: 20021214
Last Updated on STN: 20030618

Entered Medline: 20030617

AB Cathepsin F is a cysteine protease believed to be involved in the antigen-presenting process of the class II major histocompatibility complex (MHC-II) in macrophages. It has been expressed, purified and crystallized. A complete data set to a resolution of 2.5 A has been collected at room temperature. The Laue group was determined to be orthorhombic, space group P2(1)2(1)2, with unit-cell parameters a = 68.9, b = 104.8, c = 68.5 A.

L30 ANSWER 14 OF 63 MEDLINE on STN
ACCESSION NUMBER: 2002174812 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 11906282
TITLE: Molecular dynamics and free energy analyses of cathepsin D-inhibitor interactions: insight into structure-based ligand design.
AUTHOR: Huo Shuanghong; Wang Junmei; Cieplak Piotr; Kollman Peter A; Kuntz Irwin D
CORPORATE SOURCE: Department of Pharmaceutical Chemistry, University of California, San Francisco, 513 Parnassus Avenue, San Francisco, California 94143-0446, USA.
CONTRACT NUMBER: 1-R03 TW01234-01 (FIC)
GM-29072 (NIGMS)
GM-31497 (NIGMS)
P41RR-01081 (NCRR)
SOURCE: Journal of medicinal chemistry, (2002 Mar 28) 45 (7) 1412-9.
Journal code: 9716531. ISSN: 0022-2623.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200204
ENTRY DATE: Entered STN: 20020322
Last Updated on STN: 20020430
Entered Medline: 20020429

AB In this study, we compare the calculated and experimental binding free energies for a combinatorial library of inhibitors of cathepsin D (CatD), an aspartyl protease. Using a molecular dynamics (MD)-based, continuum solvent method (MM-PBSA), we are able to reproduce the experimental binding affinity for a set of seven inhibitors with an average error of ca. 1 kcal/mol and a correlation coefficient of 0.98. By comparing the dynamical conformations of the inhibitors complexed with CatD with the initial conformations generated by CombiBuild (University of California, San Francisco, CA, 1995), we have found that the docking conformation observed in an X-ray structure of one peptide inhibitor bound to CatD (Proc. Natl. Acad. Sci. U.S.A. 1993, 90, 6796-6800) is in good agreement with our MD simulation. However, the DOCK scoring function, based on intermolecular van der Waals and electrostatics, using a distance-dependent dielectric constant (J. Comput. Chemical 1992, 13, 505-524), poorly reproduces the trend of experimental binding affinity for these inhibitors. Finally, the use of PROFEC (J. Comput.-Aided Mol. Des. 1998, 12, 215-227) analysis allowed us to identify two possible substitutions to improve the binding of one of the better inhibitors to CatD. This study offers hope that current methods of estimating the free energy of binding are accurate enough to be used in a multistep virtual screening protocol.

L30 ANSWER 15 OF 63 MEDLINE on STN
ACCESSION NUMBER: 2002466510 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 12225749
TITLE: The crystal structure of human cathepsin F and its implications for the development of novel immunomodulators.
AUTHOR: Somoza John R; Palmer James T; Ho Joseph D
CORPORATE SOURCE: Department of Medicinal and Structural Chemistry, Celera, 180 Kimball Way, 94080, South San Francisco, CA, USA..
john.somoza@elera.com
SOURCE: Journal of molecular biology, (2002 Sep 20) 322 (3) 559-68.
Journal code: 2985088R. ISSN: 0022-2836.
PUB. COUNTRY: England: United Kingdom
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
OTHER SOURCE: PDB-1M6D
ENTRY MONTH: 200210

ENTRY DATE: Entered STN: 20020913
Last Updated on STN: 20021031
Entered Medline: 20021030

AB Cathepsin F is a lysosomal cysteine protease of the papain family, and likely plays a regulatory role in processing the invariant chain that is associated with the major histocompatibility complex (MHC) class II. Evidence suggests that inhibiting cathepsin F activity will block MHC class II processing in macrophages. Consequently, inhibitors of this enzyme may be useful in treating certain diseases that involve an inappropriate or excessive immune response. We have determined the 1.7A structure of the mature domain of human cathepsin F associated with an irreversible vinyl sulfone inhibitor. This structure provides a basis for understanding cathepsin F's substrate specificity, and suggests ways of identifying potent and selective inhibitors of this enzyme.

L30 ANSWER 16 OF 63 MEDLINE on STN DUPLICATE 5
ACCESSION NUMBER: 2002148581 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 11856830
TITLE: Structure of a Cys25-->Ser mutant of human cathepsin S.
AUTHOR: Turkenburg Johan P; Lamers Marieke B A C; Brzozowski A Marek; Wright Lisa M; Hubbard Roderick E; Sturt Simone L; Williams David H
CORPORATE SOURCE: York Structural Biology Laboratory, Chemistry Department, University of York, Heslington, York YO10 5DD, England.
SOURCE: Acta crystallographica. Section D, Biological crystallography, (2002 Mar) 58 (Pt 3) 451-5. Electronic Publication: 2002-02-21.
Journal code: 9305878. ISSN: 0907-4449.
PUB. COUNTRY: Denmark
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
OTHER SOURCE: PDB-1GLO
ENTRY MONTH: 200206
ENTRY DATE: Entered STN: 20020308
Last Updated on STN: 20020619
Entered Medline: 20020618

AB Cathepsin S (EC 3.4.22.27), a cysteine proteinase of the papain superfamily, plays a critical role in the generation of a major histocompatibility complex (MHC) class II restricted T-cell response by antigen-presenting cells. Therefore, selective inhibition of this enzyme may be useful in modulating class II restricted T-cell responses in immune-related disorders such as rheumatoid arthritis, multiple sclerosis and extrinsic asthma. The three-dimensional structure at 2.2 A resolution of the active-site Cys25-->Ser mutant presented here in an unliganded state provides further insight useful for the design of selective enzyme inhibitors.

L30 ANSWER 17 OF 63 EMBASE COPYRIGHT (c) 2006 Elsevier B.V. All rights reserved on STN
ACCESSION NUMBER: 2002345470 EMBASE Full-text
TITLE: Novel protease inhibitors.
AUTHOR: Norman P.
CORPORATE SOURCE: Dr. P. Norman, Norman Consulting, 18 Pink Lane, Burnham, Buckx, SL1 8JW, United Kingdom
SOURCE: Drug News and Perspectives, (2002) Vol. 15, No. 6, pp. 372-382.
ISSN: 0214-0934 CODEN: DNPEED
COUNTRY: Spain
DOCUMENT TYPE: Journal; Conference Article
FILE SEGMENT: 030 Pharmacology
037 Drug Literature Index
LANGUAGE: English
SUMMARY LANGUAGE: English
ENTRY DATE: Entered STN: 20021017
Last Updated on STN: 20021017

AB The Third RSC-SCI Symposium on Proteinase Inhibitor Design: Proteinase 2002, held May 13-14, 2002, in London, United Kingdom, drew an audience of about 140 scientists to the SCI's Belgrave Square headquarters to hear 17 speakers address various aspects of this theme. There was considerable emphasis placed upon the use of X-ray crystallography of enzyme-inhibitor complex as an integral tool in the design of improved protease inhibitors. This biennial meeting has established a reputation for being a key forum for the disclosure of

new compounds, and this year's meeting was no exception, with much of the emphasis placed on novel inhibitors of either serine or cysteine proteases. .COPYRGT. 2002 Prous Science. All rights reserved.

L30 ANSWER 18 OF 63 EMBASE COPYRIGHT (c) 2006 Elsevier B.V. All rights reserved on STN

ACCESSION NUMBER: 2002304948 EMBASE Full-text
TITLE: The cell biology of antigen presentation.
AUTHOR: Hudson A.W.; Ploegh H.L.
CORPORATE SOURCE: H.L. Ploegh, Department of Pathology, Harvard Medical School, 200 Longwood Avenue, Boston, MA 02115, United States. ploegh@hms.harvard.edu
SOURCE: Experimental Cell Research, (2002) Vol. 272, No. 1, pp. 1-7.
Refs: 33
ISSN: 0014-4827 CODEN: ECREAL
COUNTRY: United States
DOCUMENT TYPE: Journal; (Short Survey)
FILE SEGMENT: 026 Immunology, Serology and Transplantation
029 Clinical Biochemistry
LANGUAGE: English
ENTRY DATE: Entered STN: 20020913
Last Updated on STN: 20020913
DATA NOT AVAILABLE FOR THIS ACCESSION NUMBER

L30 ANSWER 19 OF 63 MEDLINE on STN

ACCESSION NUMBER: 2001567891 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 11495896
TITLE: Hemoglobin-degrading, aspartic proteases of blood-feeding parasites: substrate specificity revealed by homology models.
AUTHOR: Brinkworth R I; Prociv P; Loukas A; Brindley P J
CORPORATE SOURCE: Institute of Molecular Biosciences and Department of Microbiology and Parasitology, University of Queensland, Brisbane, Queensland 4072, Australia.
SOURCE: Journal of biological chemistry, (2001 Oct 19) 276 (42) 38844-51. Electronic Publication: 2001-08-08.
Journal code: 2985121R. ISSN: 0021-9258.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200112
ENTRY DATE: Entered STN: 20011025
Last Updated on STN: 20030105
Entered Medline: 20011204

AB Blood-feeding parasites, including schistosomes, hookworms, and malaria parasites, employ aspartic proteases to make initial or early cleavages in ingested host hemoglobin. To better understand the substrate affinity of these aspartic proteases, sequences were aligned with and/or three-dimensional, molecular models were constructed of the cathepsin D-like aspartic proteases of schistosomes and hookworms and of plasmepsins of Plasmodium falciparum and Plasmodium vivax, using the structure of human cathepsin D bound to the inhibitor pepstatin as the template. The catalytic subsites S5 through S4' were determined for the modeled parasite proteases. Subsequently, the crystal structure of mouse renin complexed with the nonapeptidyl inhibitor t-butyl-CO-His-Pro-Phe-His-Leu [CHOHCH(2)]Leu-Tyr- Tyr-Ser- NH(2) (CH-66) was used to build homology models of the hemoglobin-degrading peptidases docked with a series of octapeptide substrates. The modeled octapeptides included representative sites in hemoglobin known to be cleaved by both Schistosoma japonicum cathepsin D and human cathepsin D, as well as sites cleaved by one but not the other of these enzymes. The peptidase-octapeptide substrate models revealed that differences in cleavage sites were generally attributable to the influence of a single amino acid change among the P5 to P4' residues that would either enhance or diminish the enzymatic affinity. The difference in cleavage sites appeared to be more profound than might be expected from sequence differences in the enzymes and hemoglobins. The findings support the notion that selective inhibitors of the hemoglobin-degrading peptidases of blood-feeding parasites at large could be developed as novel anti-parasitic agents.

L30 ANSWER 20 OF 63 SCISEARCH COPYRIGHT (c) 2006 The Thomson Corporation on

STN
ACCESSION NUMBER: 2002:19845 SCISEARCH Full-text
THE GENUINE ARTICLE: 505UF
TITLE: Diaquabis(4,4 '-bipyridine)copper(II) di(o-sulfobenzimidate) dichloromethane solvate, a two-dimensional Cu-4(4,4 '-C5H4NC5H4N)(4) rhombic grid clathrating guest dichloromethane
AUTHOR: Naumov P (Reprint); Jovanovski G; Hanna J V; Razak I A; Chantrapromma S; Fun H K; Ng S W
CORPORATE SOURCE: Sv Kiril & Metodij Univ, Inst Chem, Fac Sci, POB 162, MK-91001 Skopje, Macedonia (Reprint); Sv Kiril & Metodij Univ, Inst Chem, Fac Sci, MK-91001 Skopje, Macedonia; Australian Nucl Sci & Technol Org, Lucas Hts Res Labs, Menai, NSW 2234, Australia; Univ Sains Malaysia, Sch Phys, Xray Crystallog Unit, George Town 11800, Malaysia; Prince Songkla Univ, Fac Sci, Dept Chem, Songkhla 90112, Thailand; Univ Malaya, Inst Postgrad Studies, Kuala Lumpur 50603, Malaysia
COUNTRY OF AUTHOR: Macedonia; Australia; Malaysia; Thailand
SOURCE: INORGANIC CHEMISTRY COMMUNICATIONS, (DEC 2001) Vol. 4, No. 12, pp. 766-768.
ISSN: 1387-7003.
PUBLISHER: ELSEVIER SCIENCE BV, PO BOX 211, 1000 AE AMSTERDAM, NETHERLANDS.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 29
ENTRY DATE: Entered STN: 11 Jan 2002
Last Updated on STN: 11 Jan 2002
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB In the crystal structure of bis(4,4'- bipyridine)diaquacopper(II) di(o-sulfobenzimidate) dichloromethane solvate, the host polycationic [Cu(4,4'-C5H4NC5H4N)(2)(H2O)(2)](infinity) rhombic grids stack over each other 8.16 Angstrom apart along the c-axis of the orthorhombic Pbcn unit cell. The Cu-4 (4,4'-bpy), rhombus clathrating a disordered dichloromethane molecule has a copper atom at the corner and the spacer heterocycle with pyridyl rings twisted by 21.8(2)degrees, as its side. The anions occupy the space between the layers; the grids interact with each other indirectly through water-anion hydrogen bonds [(OO)-O-... = 2.766(4); (ON)-N-... = 3.061(4) Angstrom]. The structure sets a remarkable example of potentials born by the polyfunctional o-sulfobenzimidate moiety for construction of unusual architectures. (C) 2001 Elsevier Science B.V.

L30 ANSWER 21 OF 63 SCISEARCH COPYRIGHT (c) 2006 The Thomson Corporation on STN
ACCESSION NUMBER: 2001:389585 SCISEARCH Full-text
THE GENUINE ARTICLE: 430JB
TITLE: The three-dimensional structure of human granzyme B compared to caspase-3, key mediators of cell death with cleavage specificity for aspartic acid in P1
AUTHOR: Rotonda J (Reprint); Garcia-Calvo M; Bull H G; Geissler W M; McKeever B M; Willoughby C A; Thornberry N A; Becker J W
CORPORATE SOURCE: Merck & Co Inc, Merck Sharp & Dohme Res Labs, Dept Endocrinol & Chem Biol, POB 2000, Rahway, NJ 07065 USA (Reprint); Merck & Co Inc, Merck Sharp & Dohme Res Labs, Dept Endocrinol & Chem Biol, Rahway, NJ 07065 USA; Merck & Co Inc, Merck Sharp & Dohme Res Labs, Dept Mol Endocrinol, Rahway, NJ 07065 USA; Merck & Co Inc, Merck Sharp & Dohme Res Labs, Dept Med Chem, Rahway, NJ 07065 USA
COUNTRY OF AUTHOR: USA
SOURCE: CHEMISTRY & BIOLOGY, (APR 2001) Vol. 8, No. 4, pp. 357-368
ISSN: 1074-5521.
PUBLISHER: CURRENT BIOLOGY LTD, 84 THEOBALDS RD, LONDON WC1X 8RR, ENGLAND.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 48
ENTRY DATE: Entered STN: 25 May 2001
Last Updated on STN: 25 May 2001

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB Background: Granzyme B, one of the most abundant granzymes in cytotoxic T-lymphocyte (CTL) granules, and members of the caspase (cysteine aspartyl proteinases) family have a unique cleavage specificity for aspartic acid in P1 and play critical roles in the biochemical events that culminate in cell death. Results: We have determined the three-dimensional structure of the complex of the human granzyme B with a potent tetrapeptide aldehyde inhibitor. The Asp-specific S1 subsite of human granzyme B is significantly larger and less charged than the corresponding Asp-specific site in the apoptosis-promoting caspases, and also larger than the corresponding subsite in rat granzyme B. Conclusions: The above differences account for the variation in substrate specificity among granzyme B, other serine proteases and the caspases, and enable the design of specific inhibitors that can probe the physiological functions of these proteins and the disease states with which they are associated. (C) 2001 Published by Elsevier Science Ltd.

L30 ANSWER 22 OF 63 SCISEARCH COPYRIGHT (c) 2006 The Thomson Corporation on STN

ACCESSION NUMBER: 2001:281141 SCISEARCH Full-text
THE GENUINE ARTICLE: 415WH
TITLE: Outer-sphere coordination, N-coordination and O-coordination of the deprotonated saccharin in copper(II) saccharinato complexes. Implications for the saccharinato carbonyl stretching frequency
AUTHOR: Naumov P (Reprint); Jovanovski G; Drew M G B; Ng S W
CORPORATE SOURCE: Tokyo Inst Technol, Dept Chem & Mat Sci, Ohashi Lab, Meguro Ku, 2-12-1 Ookayama, Tokyo 1528551, Japan (Reprint); Sv Kiril Metodij Univ, Fac Sci, Inst Chem, MK-1001 Skopje, Macedonia; Univ Reading, Dept Chem, Reading RG6 2AD, Berks, England; Univ Malaya, Inst Postgrad Studies & Res, Kuala Lumpur 50603, Malaysia
COUNTRY OF AUTHOR: Japan; Macedonia; England; Malaysia
SOURCE: INORGANICA CHIMICA ACTA, (19 MAR 2001) Vol. 314, No. 1-2, pp. 154-162.
ISSN: 0020-1693.
PUBLISHER: ELSEVIER SCIENCE SA, PO BOX 564, 1001 LAUSANNE, SWITZERLAND.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 52
ENTRY DATE: Entered STN: 13 Apr 2001
Last Updated on STN: 13 Apr 2001

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB Tetraaquabis(o-sulfobenzimidato-N)copper(II) reacts with neutral N-heterocycles to form complexes in which the o-sulfobenzimide (saccharin) entity interacts directly with the copper atom (through either the endocyclic nitrogen atom or the exocyclic oxygen atom) or indirectly, through coordinated water molecules. With 4-aminopyridine, it yields diaquatetrakis(4-aminopyridine)copper(II)di(o-sulfobenzimidate)dihydrate, whose metal atom shows trans-N4O2 octahedral coordination. The o-sulfobenzimidate anions interact with the copper atom through the coordinated water molecules, and they link with the lattice water molecules to furnish three-dimensional network architecture. The reagent when treated with pyrazole affords tetrakis(pyrazole)bis[1,2- benzisothiazolyl-3-olato 1,1-dioxide]copper(II); in this neutral compound, the metal atom and the o-sulfobenzimidate moieties are linked by covalent copper-oxygen bonds. The aqua complex with di-2-pyridylamine has the copper atom in a square-pyramidal configuration: one of the o-sulfobenzimidate ligands binds through its nitrogen atom whereas the other binds through the exocyclic oxygen atom in aqua(di-2-pyridylamine)[1,2-benzisothiazolyl-3-olato 1,1-dioxide](o- sulfobenzimidato-N)copper(II), which adopts a linear hydrogen-bonded chain motif. When treated with nicotinamide, tetraaquabis(o-sulfobenzimidato- N)copper(II) affords a monohydrated di(nicotinic acid) adduct, the amide group being oxidized to a carboxylic group. Tn this square-pyramidal complex, the molecules are linked by hydrogen bonds involving the two carboxylic acid ends into a linear chain that propagates along the a-e diagonal of the unit cell. The coordination mode of the o-sulfobenzimidate entities in the complexes is reflected in the stretching frequencies of the carbonyl groups, the respective band(s) being blue-shifted for N-coordination and red-shifted for O-coordination relatively to the o-sulfobenzimidate ions, leading to the frequency order N-coordinated > uncoordinated > O-coordinated. These shifts

should be considered in vibrational frequency versus bond order correlations. (C) 2001 Elsevier Science B.V. All rights reserved.

L30 ANSWER 23 OF 63 MEDLINE on STN
ACCESSION NUMBER: 2000302831 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 10841792
TITLE: Peptide and peptide mimetic inhibitors of antigen presentation by HLA-DR class II MHC molecules. Design, structure-activity relationships, and X-ray crystal structures.
AUTHOR: Bolin D R; Swain A L; Sarabu R; Berthel S J; Gillespie P; Huby N J; Makofske R; Orzechowski L; Perrotta A; Toth K; Cooper J P; Jiang N; Falcioni F; Campbell R; Cox D; Gaizband D; Belunis C J; Vidovic D; Ito K; Crowther R; Kammlott U; Zhang X; Palermo R; Weber D; Guenot J; Nagy Z; Olson G L
CORPORATE SOURCE: Roche Research Center, Hoffmann-La Roche Inc., Nutley, New Jersey 07110, USA.
SOURCE: Journal of medicinal chemistry, (2000 Jun 1) 43 (11) 2135-48.
Journal code: 9716531. ISSN: 0022-2623.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200007
ENTRY DATE: Entered STN: 20000720
Last Updated on STN: 20000720
Entered Medline: 20000707

AB Molecular features of ligand binding to MHC class II HLA-DR molecules have been elucidated through a combination of peptide structure-activity studies and structure-based drug design, resulting in analogues with nanomolar affinity in binding assays. Stabilization of lead compounds against cathepsin B cleavage by N-methylation of noncritical backbone NH groups or by dipeptide mimetic substitutions has generated analogues that compete effectively against protein antigens in cellular assays, resulting in inhibition of T-cell proliferation. Crystal structures of four ternary complexes of different peptide mimetics with the rheumatoid arthritis-linked MHC DRB10401 and the bacterial superantigen SEB have been obtained. Peptide-sugar hybrids have also been identified using a structure-based design approach in which the sugar residue replaces a dipeptide. These studies illustrate the complementary roles played by phage display library methods, peptide analogue SAR, peptide mimetics substitutions, and structure-based drug design in the discovery of inhibitors of antigen presentation by MHC class II HLA-DR molecules.

L30 ANSWER 24 OF 63 SCISEARCH COPYRIGHT (c) 2006 The Thomson Corporation on STN
ACCESSION NUMBER: 2000:881910 SCISEARCH Full-text
THE GENUINE ARTICLE: 373QH
TITLE: X-ray structures of five renin inhibitors bound to saccharopepsin: Exploration of active-site specificity
AUTHOR: Cronin N B; Badasso M O; Tickle I J; Dreyer T; Hoover D J; Rosati R L; Humblet C C; Lunney E A; Cooper J B (Reprint)
CORPORATE SOURCE: Univ Southampton, Sch Biol Sci, Div Biochem & Mol Biol, Southampton SO16 7PX, Hants, England (Reprint); Warner Lambert Co, Parke Davis Pharmaceut Res, Dept Chem, Ann Arbor, MI 48106 USA; Warner Lambert Co, Parke Davis Pharmaceut Res, Dept Pharmacol, Ann Arbor, MI 48106 USA; Univ London Birkbeck Coll, Dept Crystallog, London WC1E 7HX, England; Univ Minnesota, Dept Microbiol & Oral Sci, Minneapolis, MN 55455 USA; Carlsberg Lab, Dept Chem, DK-2500 Copenhagen, Denmark; Pfizer Inc, Div Cent Res, Dept Med Chem, Groton, CT 06340 USA
COUNTRY OF AUTHOR: England; USA; Denmark
SOURCE: JOURNAL OF MOLECULAR BIOLOGY, (10 NOV 2000) Vol. 303, No. 5, pp. 745-760.
ISSN: 0022-2836.
PUBLISHER: ACADEMIC PRESS LTD, 24-28 OVAL RD, LONDON NW1 7DX, ENGLAND
DOCUMENT TYPE: Article; Journal

LANGUAGE: English
REFERENCE COUNT: 44
ENTRY DATE: Entered STN: 2000
Last Updated on STN: 2000
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB Saccharopepsin is a vacuolar aspartic proteinase involved in activation of a number of hydrolases. The enzyme has great structural homology to mammalian aspartic proteinases including human renin and we have used it as a model system to study the binding of renin inhibitors by X-ray crystallography. Five medium-to-high resolution structures of saccharopepsin complexed with transition-state analogue renin inhibitors were determined. The structure of a cyclic peptide inhibitor (PD-129,541) complexed with the proteinase was solved to 2.5 Angstrom, resolution. This inhibitor has low affinity for human renin yet binds very tightly to the yeast proteinase (K-i = 4 nM). The high affinity of this inhibitor can be attributed to its bulky cyclic moiety spanning P-2-P-3' and other residues that appear to optimally fit the binding sub-sites of the enzyme. Superposition of the saccharopepsin structure on that of renin showed that a movement of the loop 286-301 relative to renin facilitates tighter binding of this inhibitor to saccharopepsin. Our 2.8 Angstrom resolution structure of the complex with CP-108,420 shows that its benzimidazole P-3 replacement retains one of the standard hydrogen bonds that normally involve the inhibitor's main-chain. This suggests a non-peptide lead in overcoming the problem of susceptible peptide bonds in the design of aspartic proteinase inhibitors. CP-72,647 which possesses a basic histidine residue at P-2, has a high affinity for renin (K-i = 5 nM) but proves to be a poor inhibitor for saccharopepsin (K-i = 3.7 muM) This may stem from the fact that the histidine residue would not bind favourably with the predominantly hydrophobic S-2 sub-site of saccharopepsin. (C) 2000 Academic Press.

L30 ANSWER 25 OF 63 MEDLINE on STN DUPLICATE 6
ACCESSION NUMBER: 2000206743 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 10739956
TITLE: Substrate specificity of bovine cathepsin B and its inhibition by CA074, based on crystal structure refinement of the complex.
AUTHOR: Yamamoto A; Tomoo K; Hara T; Murata M; Kitamura K; Ishida T
CORPORATE SOURCE: Department of Physical Chemistry, Osaka University of Pharmaceutical Sciences, Nasahara, Takatsuki, Japan.
SOURCE: Journal of biochemistry, (2000 Apr) 127 (4) 635-43.
Journal code: 0376600. ISSN: 0021-924X.
PUB. COUNTRY: Japan
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200007
ENTRY DATE: Entered STN: 20000810
Last Updated on STN: 20000810
Entered Medline: 20000727

AB The crystal structure of the bovine spleen cathepsin B (BSCB)-CA074 complex was refined to R = 0.152 using X- ray diffraction data up to 2.18 A resolution. BSCB is characterized by an extra Cys148-Cys252 disulfide bridge, as compared with rat and human CBs. Although the crystal structures of these enzymes showed similar overall folding, a difference was observed in the occluding loop, a structural element specific only to CB. Comparison of the torsion angles indicated the different flexibilities of their loop structures. The oxirane C6 atom of CA074 was covalently bonded to the Cys29 S(gamma) atom (C3-S(gamma)=1.81 A), where the S-configuration was transformed to the R-form. Concerning the oxirane carbon atom that participates in the covalent bonding with the Cys residue, an acceptable rule has been proposed. The substrate specificities at the Sn (n = 1-3) and Sn' (n=1 and 2) subsites of CB, together with the interaction features as to CA074, have been discussed in comparison with the crystal structure of the papain-CA028 (a CA074-related inhibitor) complex .

L30 ANSWER 26 OF 63 MEDLINE on STN
ACCESSION NUMBER: 2001032015 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 10849752
TITLE: Development and validation of homology models of human cathepsins K, S, H, and F.
AUTHOR: Fengler A; Brandt W
CORPORATE SOURCE: Department of Biochemistry and Biotechnology, Martin Luther University Halle-Wittenberg, Saale, Germany.

SOURCE: Advances in experimental medicine and biology, (2000) 477 255-60.
Journal code: 0121103. ISSN: 0065-2598.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200011
ENTRY DATE: Entered STN: 20010322
Last Updated on STN: 20010322
Entered Medline: 20001120

AB Models of the tertiary structures of cathepsins K, S, H, and F were constructed by using homology protein modelling methods and refinements by interactive graphics and energy minimisation. The predicted structures yield information regarding their substrate binding sites and indicate the residues surrounding these sites. The ligand binding sites were characterised and compared with each other by means of calculated molecular electrostatic surface potentials. This will allow designing and development of new ligands specific for these cathepsins in future investigations.

L30 ANSWER 27 OF 63 MEDLINE on STN
ACCESSION NUMBER: 1999146897 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 10022822
TITLE: Crystal structure of MHC class II-associated p41 Ii fragment bound to cathepsin L reveals the structural basis for differentiation between cathepsins L and S.
AUTHOR: Guncar G; Pungercic G; Klemencic I; Turk V; Turk D
CORPORATE SOURCE: Department of Biochemistry and Molecular Biology, Jozcaronef Stefan Institute, Jamova 39, SLO-1000 Ljubljana, Slovenia.
SOURCE: EMBO journal, (1999 Feb 15) 18 (4) 793-803.
Journal code: 8208664. ISSN: 0261-4189.
PUB. COUNTRY: ENGLAND: United Kingdom
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199904
ENTRY DATE: Entered STN: 19990511
Last Updated on STN: 20020420
Entered Medline: 19990426

AB The lysosomal cysteine proteases cathepsins S and L play crucial roles in the degradation of the invariant chain during maturation of MHC class II molecules and antigen processing. The p41 form of the invariant chain includes a fragment which specifically inhibits cathepsin L but not S. The crystal structure of the p41 fragment, a homologue of the thyroglobulin type-1 domains, has been determined at 2.0 A resolution in complex with cathepsin L. The structure of the p41 fragment demonstrates a novel fold, consisting of two subdomains, each stabilized by disulfide bridges. The first subdomain is an alpha-helix-beta-strand arrangement, whereas the second subdomain has a predominantly beta-strand arrangement. The wedge shape and three-loop arrangement of the p41 fragment bound to the active site cleft of cathepsin L are reminiscent of the inhibitory edge of cystatins, thus demonstrating the first example of convergent evolution observed in cysteine protease inhibitors. However, the different fold of the p41 fragment results in additional contacts with the top of the R-domain of the enzymes, which defines the specificity-determining S2 and S1' substrate-binding sites. This enables inhibitors based on the thyroglobulin type-1 domain fold, in contrast to the rather non-selective cystatins, to exhibit specificity for their target enzymes.

L30 ANSWER 28 OF 63 MEDLINE on STN DUPLICATE 7
ACCESSION NUMBER: 1999134396 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 9931257
TITLE: The 2.2 A crystal structure of human chymase in complex with succinyl-Ala-Ala-Pro-Phe-chloromethylketone: structural explanation for its dipeptidyl carboxypeptidase specificity.
AUTHOR: Pereira P J; Wang Z M; Rubin H; Huber R; Bode W; Schechter N M; Strobl S
CORPORATE SOURCE: Abteilung fur Strukturforschung, Max-Planck-Institut fur Biochemie, Am Klopferspitz 18a, Martinsried, D-82152, Germany.

CONTRACT NUMBER: AR42931 (NIAMS)
HL50523 (NHLBI)
SOURCE: Journal of molecular biology, (1999 Feb 12) 286 (1) 163-73.
Journal code: 2985088R. ISSN: 0022-2836.
PUB. COUNTRY: ENGLAND: United Kingdom
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
OTHER SOURCE: PDB-1PJP
ENTRY MONTH: 199903
ENTRY DATE: Entered STN: 19990413
Last Updated on STN: 20000303
Entered Medline: 19990329

AB Human chymase (HC) is a chymotrypsin-like serine proteinase expressed by mast cells. The 2.2 A crystal structure of HC complexed to the peptidyl inhibitor, succinyl-Ala-Ala-Pro-Phe- chloromethylketone (CMK), was solved and refined to a crystallographic R-factor of 18.4 %. The HC structure exhibits the typical folding pattern of a chymotrypsin-like serine proteinase, and shows particularly similarity to rat chymase 2 (rat mast cell proteinase II) and human cathepsin G. The peptidyl-CMK inhibitor is covalently bound to the active-site residues Ser195 and His57; the peptidyl moiety juxtaposes the S1 entrance frame segment 214-217 by forming a short antiparallel beta-sheet. HC is a highly efficient angiotensin-converting enzyme. Modeling of the chymase-angiotensin I interaction guided by the geometry of the bound chloromethylketone inhibitor indicates that the extended substrate binding site contains features that may generate the dipeptidyl carboxypeptidase-like activity needed for efficient cleavage and activation of the hormone. The C-terminal carboxylate group of angiotensin I docked into the active-site cleft, with the last two residues extending beyond the active site, is perfectly localized to make a favorable hydrogen bond and salt bridge with the amide nitrogen of the Lys40-Phe41 peptide bond and with the epsilon-ammonium group of the Lys40 side-chain. This amide positioning is unique to the chymase-related proteinases, and only chymases from primates possess a Lys residue at position 40. Thus, the structure conveniently explains the preferred conversion of angiotensin I to angiotensin II by human chymase.

L30 ANSWER 29 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:479610 CAPLUS Full-text
DOCUMENT NUMBER: 129:92255
TITLE: Human factor Xa with truncated light chain and crystals thereof for use in developing antithrombotic drugs
INVENTOR(S): Chmielewska, Joanna; Lundqvist, Tomas; Mosialou, Erifili; Ogg, Derek
PATENT ASSIGNEE(S): Pharmacia & Upjohn AB, Swed.
SOURCE: PCT Int. Appl., 20 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9828412	A1	19980702	WO 1997-SE2160		19971218
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
AU 9855812	A1	19980717	AU 1998-55812		19971218
US 6069234	A	20000530	US 1997-994328		19971219
PRIORITY APPLN. INFO.:			SE 1996-4744	A	19961220
			WO 1997-SE2160	W	19971218

AB The present invention is directed to a modified coagulation factor Xa which has an improved capacity of forming crystals compared to its native form. The factor is modified by deletion of N- and/or C-terminal amino acids from the light chain. Such crystals or crystalline composition are especially useful for studies in crystalline form of the active catalytic side of factor Xa when it is complexed to a specific affinity ligand with

inhibiting characteristics. Factor Xa containing 45-138-light chain was prepared by digesting factor Xa with cathepsin G and carboxypeptidase B. This modified factor Xa has therefore lost its γ-carboxy-Glu-containing region as well as its C-terminal Arg. Crystals of the modified factor Xa complexed with inhibitor DS-9065a and uncomplexed factor Xa were obtained, X-ray diffraction patterns were produced, and the 3D structures were determined

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 30 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:546547 CAPLUS Full-text
DOCUMENT NUMBER: 129:272204
TITLE: Use of X-ray Co-crystal Structures and Molecular Modeling To Design Potent and Selective Non-peptide Inhibitors of Cathepsin K
AUTHOR(S): DesJarlais, Renee L.; Yamashita, Dennis S.; Oh, Hye-Ja; Uzinskas, Irene N.; Erhard, Karl F.; Allen, Andrew C.; Haltiwanger, R. Curtis; Zhao, Baoguang; Smith, Ward W.; Abdel-Meguid, Sherin S.; D'Alessio, Karla; Janson, Cheryl A.; McQueney, Michael S.; Tomaszek, Thaddeus A.; Levy, Mark A.; Veber, Daniel F.
CORPORATE SOURCE: Departments of Physical and Structural Chemistry Medicinal Chemistry Analytical Chemistry Structural Biology Protein Biochemistry and Molecular Recognition, SmithKline Beecham Pharmaceuticals, King of Prussia, PA, 19406, USA
SOURCE: Journal of the American Chemical Society (1998), 120(35), 9114-9115
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB By making use of X-ray crystal structures of cathepsin K/inhibitor complexes and mol. modeling, cathepsin K inhibitors of the 1,3-bis(acylamino)-2- propanone series that lack a leucinyl group have now been designed. These inhibitors are equipotent with their closest leucine-derived analogs and are selective for human cathepsin K over human cathepsins B, L, and S. To decrease the peptidic nature of our lead compound, 1,3- bis(Cbz-Leu-NH)-2-propanone 1 analogs were synthesized in which one of the Cbz-Leu groups was replaced with peptidomimetics. For instance, the 2-pyridylsulfonyl analog 2 was notable since it had increased water solubility with only a 2-fold loss in potency relative to 1. Examination of the 3-dimensional structures of cathepsin K/inhibitor complexes, obtained by X-ray crystallog., indicated several important recognition elements in our cathepsin K inhibitors including the iso-Bu side chain of the leucine, which binds in the hydrophobic S23 pocket of the enzyme and the two Cbz Ph rings, which each form aromatic-aromatic interactions, one with Tyr 67 on the unprime side and the other with Trp 184 on the prime3 side of the active site.
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 31 OF 63 MEDLINE on STN
ACCESSION NUMBER: 1998254543 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 9585570
TITLE: The role of Gly-4 of human cystatin A (stefin A) in the binding of target proteinases. Characterization by kinetic and equilibrium methods of the interactions of cystatin A Gly-4 mutants with papain, cathepsin B, and cathepsin L.
AUTHOR: Estrada S; Nycander M; Hill N J; Craven C J; Waltho J P; Bjork I
CORPORATE SOURCE: Department of Veterinary Medical Chemistry, Swedish University of Agricultural Sciences, Uppsala Biomedical Center.
SOURCE: Biochemistry, (1998 May 19) 37 (20) 7551-60.
Journal code: 0370623. ISSN: 0006-2960.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
OTHER SOURCE: PDB-1DVC; PDB-1STF
ENTRY MONTH: 199806

ENTRY DATE: Entered STN: 19980708
Last Updated on STN: 20020420
Entered Medline: 19980622

AB The importance of the evolutionarily conserved Gly-4 residue for the affinity and kinetics of interaction of cystatin A with several cysteine proteinases was assessed by site-directed mutagenesis. Even the smallest replacement, by Ala, resulted in approximately 1000-, approximately 10- and approximately 6000-fold decreased affinities for papain, cathepsin L, and cathepsin B, respectively. Substitution by Ser gave further 3-8-fold reductions in affinity, whereas the largest decreases, >10(5)-fold, were observed for mutations to Arg and Glu. The kinetics of inhibition of papain by the mutants with small side chains, Ala and Ser, were compatible with a one-step bimolecular reaction similar to that with wild-type cystatin A. The decreased affinities of these mutants for papain and cathepsin L were due exclusively to increased dissociation rate constants, but the reduced affinities for cathepsin B were due also to decreased association rate constants. The latter finding indicates that the intact N-terminal region serves as a guide directing cystatin A to the active site of cathepsin B, as has been proposed for cystatin C. The kinetics of binding of the mutants with charged side chains, Arg and Glu, to papain were consistent with a two-step binding mechanism, in which the mutant side chains are accommodated in the complex by a conformational change. The NMR solution structure of the Ala and Trp mutants showed only minor changes compared with wild-type cystatin A, indicating that the large reductions in affinity for proteinases are not due to altered structures of the mutants. Instead, a side chain larger than a hydrogen atom at position 4 affects the interaction with the proteinase most likely by interfering with the binding of the N-terminal region.

L30 ANSWER 32 OF 63 SCISEARCH COPYRIGHT (c) 2006 The Thomson Corporation on STN
ACCESSION NUMBER: 1998:537970 SCISEARCH Full-text
THE GENUINE ARTICLE: ZZ241
TITLE: Inhibition of human neutrophil elastase. 4. Design, synthesis, X-ray crystallographic analysis, and structure-activity relationships for a series of P-2-modified, orally active peptidyl pentafluoroethyl ketones
AUTHOR: Cregge R J; Durham S L; Farr R A; Gallion S L; Hare C M; Hoffman R V; Janusz M J; Kim H O; Koehl J R; Mehdi S; Metz W A (Reprint); Peet N P; Pelton J T; Schreuder H A; Sunder S; Tardif C
CORPORATE SOURCE: Hoechst Marion Roussel Inc, 2110 E Galbraith Rd, Cincinnati, OH 45215 USA (Reprint); Hoechst Marion Roussel Inc, Cincinnati, OH 45215 USA
COUNTRY OF AUTHOR: USA
SOURCE: JOURNAL OF MEDICINAL CHEMISTRY, (2 JUL 1998) Vol. 41, No. 14, pp. 2461-2480.
ISSN: 0022-2623.
PUBLISHER: AMER CHEMICAL SOC, 1155 16TH ST, NW, WASHINGTON, DC 20036 USA.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 55
ENTRY DATE: Entered STN: 1998
Last Updated on STN: 1998
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB A series of P-2-modified, orally active peptidic inhibitors of human neutrophil elastase (HNE) are reported. These pentafluoroethyl ketone-based inhibitors were designed using pentafluoroethyl ketone 1 as a model. Rational structural modifications were made at the P-3, P-2, and activating group (A(G)) portions of 1 based on structure-activity relationships (SAR) developed from in vitro (measured K-i) data and. information provided by modeling studies that docked inhibitor 1 into the active site of HNE. The modeling-based design was corroborated with X-ray crystallographic analysis of the complex between 1 and porcine pancreatic elastase (PPE) and subsequently the complex between 1 and HNE.

L30 ANSWER 33 OF 63 MEDLINE on STN
ACCESSION NUMBER: 1998318038 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 9655332
TITLE: Crystal structure of human cathepsin S.
AUTHOR: McGrath M E; Palmer J T; Bromme D; Somoza J R

CORPORATE SOURCE: Axys Pharmaceuticals, Inc., South San Francisco, California 94080, USA.. mcgrath@arris.com
SOURCE: Protein science : a publication of the Protein Society, (1998 Jun) 7 (6) 1294-302.
Journal code: 9211750. ISSN: 0961-8368.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199809
ENTRY DATE: Entered STN: 19980910
Last Updated on STN: 19980910
Entered Medline: 19980901

AB We have determined the 2.5 A structure (Rcryst = 20.5%, Rfree = 28.5%) of a complex between human cathepsin S and the potent, irreversible inhibitor 4-morpholinecarbonyl-Phe-hPhe-vinyl sulfone-phenyl. Noncrystallographic symmetry averaging and other density modification techniques were used to improve electron density maps which were nonoptimal due to systematically incomplete data. Methods that reduce the number of parameters were implemented for refinement. The refined structure shows cathepsin S to be similar to related cysteine proteases such as papain and cathepsins K and L. As expected, the covalently-bound inhibitor is attached to the enzyme at Cys 25, and enzyme binding subsites S3-S1' are occupied by the respective inhibitor substituents. A somewhat larger S2 pocket than what is found in similar enzymes is consistent with the broader specificity of cathepsin S at this site, while Lys 61 in the S3 site may offer opportunities for selective inhibition of this enzyme. The presence of Arg 137 in the S1' pocket, and proximal to Cys 25 may have implications not only for substrate specificity C-terminal to the scissile bond, but also for catalysis.

L30 ANSWER 34 OF 63 SCISEARCH COPYRIGHT (c) 2006 The Thomson Corporation on STN
ACCESSION NUMBER: 1998:620942 SCISEARCH Full-text
THE GENUINE ARTICLE: 110NJ
TITLE: Sheep mast-cell proteinases-1 and -3: cDNA cloning, primary structure and molecular modelling of the enzymes and further studies on substrate specificity
AUTHOR: McAleese S M; Pemberton A D (Reprint); McGrath M E; Huntley J F; Miller H R P
CORPORATE SOURCE: Univ Edinburgh, Dept Vet Clin Studies, Easter Bush Vet Ctr, Roslin EH25 9RG, Midlothian, Scotland (Reprint); Axys Pharmaceut Inc, S San Francisco, CA 94080 USA; Int Res Ctr, Moredun Res Inst, Penicuik EH26 0PZ, Midlothian, Scotland
COUNTRY OF AUTHOR: Scotland; USA
SOURCE: BIOCHEMICAL JOURNAL, (1 AUG 1998) Vol. 333, Part 3, pp. 801-809.
ISSN: 0264-6021.
PUBLISHER: PORTLAND PRESS, 59 PORTLAND PLACE, LONDON W1N 3AJ, ENGLAND
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 42
ENTRY DATE: Entered STN: 1998
Last Updated on STN: 1998
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB Sheep mast-cell proteinase-1 (sMCP-1) is a serine proteinase expressed predominantly by mucosal mast cells, with specificity for cleavage C-terminal to basic and hydrophobic amino acid residues. A cDNA encoding sMCP-1 has been cloned using reverse transcriptase (RT)-PCR. It appears to be translated as a pre-proenzyme with a 17-amino-acid signal peptide, a basic 2-amino-acid propeptide and a 226-amino-acid catalytic domain. A second cDNA, encoding a serine proteinase 90% identical with sMCP-1, was also cloned and named sMCP-3. Molecular models were constructed for both enzymes using coordinates for the refined X -ray structures of human cathepsin G, chymase and rat mast-cell proteinase-2. The model for sMCP-1 suggests that the acidic Asp-226 side chain extends into the substrate-binding pocket, hydrogen-bonding with Ser-190 on the opposite side and bisecting the pocket. The location of an acidic moiety in this position would favour interaction with basic substrate residues and binding of aromatic residues is rationalized by interaction of the positively charged equatorial plane with Asp-226. The balance between chymotryptic and tryptic activities of sMCP-1 was found to be sensitive to salt concentration, with increasing univalent cation concentration favouring

chymotryptic activity relative to the tryptic. Using a peptide substrate representing residues 36-59 of the human thrombin receptor, increasing salt concentration favoured cleavage at Phe-43 rather than at Arg-41.

L30 ANSWER 35 OF 63 MEDLINE on STN
ACCESSION NUMBER: 97185906 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 9033587
TITLE: Crystal structure of human cathepsin K complexed with a potent inhibitor.
AUTHOR: McGrath M E; Klaus J L; Barnes M G; Bromme D
SOURCE: Nature structural biology, (1997 Feb) 4 (2) 105-9. Journal code: 9421566. ISSN: 1072-8368.
PUB. COUNTRY: United States
DOCUMENT TYPE: Letter
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199703
ENTRY DATE: Entered STN: 19970327
Last Updated on STN: 19970327
Entered Medline: 19970320

L30 ANSWER 36 OF 63 SCISEARCH COPYRIGHT (c) 2006 The Thomson Corporation on STN
ACCESSION NUMBER: 1997:559033 SCISEARCH Full-text
THE GENUINE ARTICLE: XM342
TITLE: Engineering of porcine pepsin - Alteration of S-1 substrate specificity of pepsin to those of fungal aspartic proteinases by site-directed mutagenesis
AUTHOR: Shintani T (Reprint); Nomura K; Ichishima E
CORPORATE SOURCE: TOHOKU UNIV, FAC AGR, DEPT APPL BIOL CHEM, LAB MOL ENZYMOL, AOBA KU, SENDAI, MIYAGI 981, JAPAN
COUNTRY OF AUTHOR: JAPAN
SOURCE: JOURNAL OF BIOLOGICAL CHEMISTRY, (25 JUL 1997) Vol. 272, No. 30, pp. 18855-18861. ISSN: 0021-9258.
PUBLISHER: AMER SOC BIOCHEMISTRY MOLECULAR BIOLOGY INC, 9650 ROCKVILLE PIKE, BETHESDA, MD 20814.
DOCUMENT TYPE: Article; Journal
FILE SEGMENT: LIFE
LANGUAGE: English
REFERENCE COUNT: 47
ENTRY DATE: Entered STN: 1997
Last Updated on STN: 1997
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB The S-1 substrate specificity of porcine pepsin has been altered to resemble that of fungal aspartic proteinase with preference for a basic amino acid residue in P-1 by site directed mutagenesis. On the basis of primary and tertiary structures of aspartic proteinases, the active site-flap mutants of porcine pepsin were constructed, which involved the replacement of Thr-77 by Asp (T77D), the insertion of Ser between Gly-78 and Ser-79 (G78(S)S79), and the double mutation (T77D/G78(S)S79). The specificities of the mutants were determined using p-nitrophenylalanine- based substrates containing a Phe or Lys residue at the P-1 position. The double mutant cleaved the Lys-Phe(4-NO2) bonds, while wild-type enzyme digested other bonds. In addition, the pH dependence of hydrolysis of Lys-containing substrates by the double mutant indicates that the interactions between Asp-77 of the mutant and P-1 Lys contribute to the transition state stabilization. The double mutant was also able to activate bovine trypsinogen to trypsin by the selective cleavage of the Lys(6)-Ile(7) bond of trypsinogen. Results of this study suggest that the structure of the active site flap contributes to the S-1 substrate specificity for basic amino acid residues in aspartic proteinases.

L30 ANSWER 37 OF 63 MEDLINE on STN DUPLICATE 8
ACCESSION NUMBER: 97377017 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 9233788
TITLE: Crystal structure of a deubiquitinating enzyme (human UCH-L3) at 1.8 A resolution.
AUTHOR: Johnston S C; Larsen C N; Cook W J; Wilkinson K D; Hill C P
CORPORATE SOURCE: Biochemistry Department, University of Utah, Salt Lake City

84132, USA.
CONTRACT NUMBER: 5-T32-GM08573 (NIGMS)
GM30308 (NIGMS)
GM50163 (NIGMS)
+
SOURCE: EMBO journal, (1997 Jul 1) 16 (13) 3787-96.
Journal code: 8208664. ISSN: 0261-4189.
PUB. COUNTRY: ENGLAND: United Kingdom
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
OTHER SOURCE: SWISSPROT-P09936; SWISSPROT-P15374; SWISSPROT-P35122; SWISSPROT-P35127
ENTRY MONTH: 199709
ENTRY DATE: Entered STN: 19970916
Last Updated on STN: 19970916
Entered Medline: 19970902

AB Ubiquitin C-terminal hydrolases catalyze the removal of adducts from the C-terminus of ubiquitin. We have determined the crystal structure of the recombinant human Ubiquitin C-terminal Hydrolase (UCH-L3) by X-ray crystallography at 1.8 A resolution. The structure is comprised of a central antiparallel beta-sheet flanked on both sides by alpha-helices. The beta-sheet and one of the helices resemble the well-known papain-like cysteine proteases, with the greatest similarity to cathepsin B. This similarity includes the UCH-L3 active site catalytic triad of Cys95, His169 and Asp184, and the oxyanion hole residue Gln89. Papain and UCH-L3 differ, however, in strand and helix connectivity, which in the UCH-L3 structure includes a disordered 20 residue loop (residues 147-166) that is positioned over the active site and may function in the definition of substrate specificity. Based upon analogy with inhibitor complexes of the papain-like enzymes, we propose a model describing the binding of ubiquitin to UCH-L3. The UCH-L3 active site cleft appears to be masked in the unliganded structure by two different segments of the enzyme (residues 9-12 and 90-94), thus implying a conformational change upon substrate binding and suggesting a mechanism to limit non-specific hydrolysis.

L30 ANSWER 38 OF 63 SCISEARCH COPYRIGHT (c) 2006 The Thomson Corporation on STN
ACCESSION NUMBER: 1997:365550 SCISEARCH Full-text
THE GENUINE ARTICLE: WY022
TITLE: Binding mode of CA074, a specific irreversible inhibitor, to bovine cathepsin B as determined by X -ray crystal analysis of the complex
AUTHOR: Yamamoto A (Reprint); Hara T; Tomoo K; Ishida T; Fujii T; Hata Y; Murata M; Kitamura K
CORPORATE SOURCE: OSAKA UNIV PHARMACEUT SCI, TAKATSUKI, OSAKA 56911, JAPAN; KYOTO UNIV, INST CHEM RES, UJI, KYOTO 611, JAPAN; TAISHO PHARMACEUT CO LTD, RES CTR, OMIYA, SAITAMA 330, JAPAN
COUNTRY OF AUTHOR: JAPAN
SOURCE: JOURNAL OF BIOCHEMISTRY, (MAY 1997) Vol. 121, No. 5, pp. 974-977.
ISSN: 0021-924X.
PUBLISHER: JAPANESE BIOCHEMICAL SOC, ISHIKAWA BLDG-3F, 25-16 HONGO-5-CHOME, BUNKYO-KU, TOKYO 113, JAPAN.
DOCUMENT TYPE: Article; Journal
FILE SEGMENT: LIFE
LANGUAGE: English
REFERENCE COUNT: 24
ENTRY DATE: Entered STN: 1997
Last Updated on STN: 1997
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB The binding mode of CA074 [N-(L-3-trans-propylcarbamoyl-oxirane-2- carbonyl)-L-isoleucyl-L-proline] , a specific irreversible inhibitor, to bovine spleen cathepsin B was elucidated by X- ray crystal structure analysis of the complex at 2.2 Angstrom resolution (conventional R=0.185), Inconsistently with our model used for the development of CA074, the L-isoleucyl-L-proline and propylcarbamoyl moieties are located at the S' and S subsites respectively, This unexpected binding is primarily due to (i) similar extended chain conformations (due to the same S configurations) at the oxirane C2 and C3 atoms of CA074 and (ii) the just fit formation of double hydrogen bonds between the carboxyl oxygens of L-proline and the imidazole nitrogens of His-110 and His-ill residues (these residues are missing in papain, the tertiary structure of which was used for the design of CA074), The

oxirane C3 atom possessing the P' substituent is covalently bound to the Cys-29 S gamma atom (C3-S gamma=1.79 Angstrom) and the S configuration is maintained. The present result will provide useful information for characterizing the substrate-specificity of cathepsin B.

L30 ANSWER 39 OF 63 MEDLINE on STN DUPLICATE 9
ACCESSION NUMBER: 97253461 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 9098904
TITLE: Expression of human cathepsin K in Pichia pastoris and preliminary crystallographic studies of an inhibitor complex.
AUTHOR: Linnevers C J; McGrath M E; Armstrong R; Mistry F R; Barnes M G; Klaus J L; Palmer J T; Katz B A; Bromme D
CORPORATE SOURCE: Arris Pharmaceutical, South San Francisco, California 94080, USA.
SOURCE: Protein science : a publication of the Protein Society, (1997 Apr) 6 (4) 919-21.
Journal code: 9211750. ISSN: 0961-8368.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199708
ENTRY DATE: Entered STN: 19970902
Last Updated on STN: 19970902
Entered Medline: 19970819

AB Cathepsin K is a cysteine protease of the papain family, which is predominantly expressed in osteoclasts, and is regarded as a key protease in bone remodeling. To facilitate structural studies of the protein, the wild-type sequence of the protease has been mutated so as to replace a potential N-glycosylation site. We have expressed the mutant human cathepsin K to 190 mg/5 L using the Pichia pastoris expression system. Cathepsin K was inactivated with the mechanism-based inhibitor, APC3328, and crystallized from magnesium formate. A 2.2 A X-ray data set has been collected on crystals belonging to space group P2(1)2(1)2(1), with a = 41.66 A, b = 51.41 A, and c = 107.72 A. There is most likely one molecule per asymmetric unit.

L30 ANSWER 40 OF 63 MEDLINE on STN DUPLICATE 10
ACCESSION NUMBER: 97286312 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 9141479
TITLE: The crystal structure of human cathepsin L complexed with E-64.
AUTHOR: Fujishima A; Imai Y; Nomura T; Fujisawa Y; Yamamoto Y; Sugawara T
CORPORATE SOURCE: Pharmaceutical Research Division, Takeda Chemical Industries, Ltd., Yodogawa-ku, Osaka, Japan..
fujishim@lab.takeda.co.jp
SOURCE: FEBS letters, (1997 Apr 21) 407 (1) 47-50.
Journal code: 0155157. ISSN: 0014-5793.
PUB. COUNTRY: Netherlands
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199706
ENTRY DATE: Entered STN: 19970612
Last Updated on STN: 20020420
Entered Medline: 19970603

AB We have determined the three dimensional structure of the complex of human cathepsin L and E-64, an irreversible inhibitor of cysteine proteases, at 2.5 A resolution. The overall structure was similar to that of other known cysteine proteases and apparently identical to the mature region of procathepsin L. The electron density for E-64 is clearly visible except for the guanidinobutane moiety. From comparison of the active sites of cathepsin L and B, we found the following: (1) The S' subsites of cathepsin L and B are totally different because of the 'occluding loop' lying on the end of the S' subsites of cathepsin B. (2) The S2 pocket of cathepsin L is shallow and narrow compared to that of cathepsin B. (3) The S3 subsites of the two enzymes are more similar than the other subsites, but cathepsin L may accommodate a more bulky group at this site. Knowledge of the active site structure of cathepsin L should be helpful for the structure-based design of potent and specific inhibitors which are of therapeutic importance.

L30 ANSWER 41 OF 63 MEDLINE on STN
ACCESSION NUMBER: 96413592 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 8816746
TITLE: Structure and inhibition of plasmepsin II, a hemoglobin-degrading enzyme from Plasmodium falciparum.
AUTHOR: Silva A M; Lee A Y; Gulnik S V; Maier P; Collins J; Bhat T N; Collins P J; Cachau R E; Luker K E; Gluzman I Y; Francis S E; Oksman A; Goldberg D E; Erickson J W
CORPORATE SOURCE: Structural Biochemistry Program, National Cancer Institute/SAIC, Frederick, MD 21702, USA.
CONTRACT NUMBER: AI 37977 (NIAID)
NO1 CO-56000 (NCI)
SOURCE: Proceedings of the National Academy of Sciences of the United States of America, (1996 Sep 17) 93 (19) 10034-9.
Journal code: 7505876. ISSN: 0027-8424.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199611
ENTRY DATE: Entered STN: 19961219
Last Updated on STN: 20000303
Entered Medline: 19961113

AB Plasmodium falciparum is the major causative agent of malaria, a disease of worldwide importance. Resistance to current drugs such as chloroquine and mefloquine is spreading at an alarming rate, and our antimalarial armamentarium is almost depleted. The malarial parasite encodes two homologous aspartic proteases, plasmepsins I and II, which are essential components of its hemoglobin-degradation pathway and are novel targets for antimalarial drug development. We have determined the crystal structure of recombinant plasmepsin II complexed with pepstatin A. This represents the first reported crystal structure of a protein from P. falciparum. The crystals contain molecules in two different conformations, revealing a remarkable degree of interdomain flexibility of the enzyme. The structure was used to design a series of selective low molecular weight compounds that inhibit both plasmepsin II and the growth of P. falciparum in culture.

L30 ANSWER 42 OF 63 MEDLINE on STN
ACCESSION NUMBER: 97051807 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 8896442
TITLE: The 1.8 A crystal structure of human cathepsin G in complex with Suc-Val-Pro-PheP-(OPh)2: a Janus-faced proteinase with two opposite specificities.
AUTHOR: Hof P; Mayr I; Huber R; Korzus E; Potempa J; Travis J; Powers J C; Bode W
CORPORATE SOURCE: Max-Planck-Institut fur Biochemie, Planegg-Martinsried, Germany.
SOURCE: EMBO journal, (1996 Oct 15) 15 (20) 5481-91.
Journal code: 8208664. ISSN: 0261-4189.
PUB. COUNTRY: ENGLAND: United Kingdom
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199612
ENTRY DATE: Entered STN: 19970128
Last Updated on STN: 20000303
Entered Medline: 19961206

AB The crystal structure of human neutrophil cathepsin G, complexed with the peptidyl phosphonate inhibitor Suc-Val-Pro-PheP-(OPh)2, has been determined to a resolution of 1.8 A using Patterson search techniques. The cathepsin G structure shows the polypeptide fold characteristic of trypsin-like serine proteinases and is especially similar to rat mast cell proteinase II. Unique to cathepsin G, however, is the presence of Glu226 (chymotrypsinogen numbering), which is situated at the bottom of the S1 specificity pocket, dividing it into two compartments. For this reason, the benzyl side chain of the inhibitor PheP residue does not fully occupy the pocket but is, instead, located at its entrance. Its positively charged equatorial edge is involved in a favourable electrostatic interaction with the negatively charged carboxylate group of Glu226. Arrangement of this Glu226 carboxylate would also allow accommodation of a Lys side chain in this S1 pocket, in agreement with the recently observed cathepsin G preference for Lys and Phe at P1. The cathepsin G complex with the covalently bound phosphonate inhibitor

mimics a tetrahedral substrate intermediate. A comparison of the Arg surface distributions of cathepsin G, leukocyte elastase and rat mast cell protease II shows no simple common recognition pattern for a mannose-6-phosphate receptor-independent targeting mechanism for sorting of these granular proteinases.

L30 ANSWER 43 OF 63 SCISEARCH COPYRIGHT (c) 2006 The Thomson Corporation on STN
ACCESSION NUMBER: 1996:834984 SCISEARCH Full-text
THE GENUINE ARTICLE: VT537
TITLE: Characterization of the S-1 subsite specificity of aspergillopepsin I by site-directed mutagenesis
AUTHOR: Shintani T (Reprint); Kobayashi M; Ichishima E
CORPORATE SOURCE: TOHOKU UNIV, FAC AGR, DEPT APPL BIOL CHEM, LAB MOL ENZYMOL, AOBA KU, SENDAI, MIYAGI 981, JAPAN
COUNTRY OF AUTHOR: JAPAN
SOURCE: JOURNAL OF BIOCHEMISTRY, (NOV 1996) Vol. 120, No. 5, pp. 974-981.
ISSN: 0021-924X.
PUBLISHER: JAPAN BIOCHEMICAL SOC, ISHIKAWA BLDG-3F 25-16 HONGO-5-CHOME, TOKYO TOKYO 113, JAPAN.
DOCUMENT TYPE: Article; Journal
FILE SEGMENT: LIFE
LANGUAGE: English
REFERENCE COUNT: 57
ENTRY DATE: Entered STN: 1996
Last Updated on STN: 1996
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB The structural determinants of Si substrate specificity of aspergillopepsin I (API; EC 3.4.23.18), an aspartic proteinase from Aspergillus saitoi, were investigated by site-directed mutagenesis. Aspartic proteinases generally favor hydrophobic amino acids at P-1 and P-1'. However, API accommodates a Lys residue at P-1, which leads to activation of trypsinogen. On the basis of amino acid sequence alignments of aspartic proteinases, Asp-76 and Ser-78 of API are conserved only in fungal enzymes with the ability to activate trypsinogen, and are located in the active-site flap. Site-directed mutants (D76N, D76E, D76S, D76T, S78A, and Delta S78) mere constructed, overexpressed in Escherichia coli cells and purified for comparative studies using natural and synthetic substrates. Substitution of Asp-76 to Ser or Thr and deletion of Ser-78, corresponding to the mammalian aspartic proteinases, caused drastic decreases in the activities towards substrates containing a basic amino acid residue at P-1. In contrast, substrates with a hydrophobic residue at P-1 were effectively hydrolyzed by each mutant enzyme. These results demonstrate that Asp-76 and Ser-78 residues on the active site flap play important roles in the recognition of a basic amino acid residue at the P-1 position.

L30 ANSWER 44 OF 63 SCISEARCH COPYRIGHT (c) 2006 The Thomson Corporation on STN
ACCESSION NUMBER: 1996:595603 SCISEARCH Full-text
THE GENUINE ARTICLE: VC335
TITLE: The crystal structure of PR3, a neutrophil serine proteinase antigen of Wegener's granulomatosis antibodies
AUTHOR: Fujinaga M (Reprint); Chernaia M M; Halenbeck R; Koths K; James M N G
CORPORATE SOURCE: UNIV ALBERTA, DEPT BIOCHEM, GRP PROTEIN STRUCT & FUNCT, MRC, EDMONTON, AB T6G 2H7, CANADA (Reprint); CHIRON CORP, CHIRON TECHNOL, EMERYVILLE, CA 94608
COUNTRY OF AUTHOR: CANADA; USA
SOURCE: JOURNAL OF MOLECULAR BIOLOGY, (16 AUG 1996) Vol. 261, No. 2, pp. 267-278.
ISSN: 0022-2836.
PUBLISHER: ACADEMIC PRESS LTD, 24-28 OVAL RD, LONDON, ENGLAND NW1 7DX
DOCUMENT TYPE: Article; Journal
FILE SEGMENT: LIFE
LANGUAGE: English
REFERENCE COUNT: 62
ENTRY DATE: Entered STN: 1996
Last Updated on STN: 1996
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB The crystal structure of PR3, a serine proteinase from the azurophilic granules of human polymorphonuclear neutrophils, has been solved by molecular replacement using the human leukocyte elastase structure. The PR3 structure has been refined to an R-factor (=Sigma parallel to F-o\-\F-c parallel to/Sigma\F-o\) of 0.201 for all data in the range of 10.0 to 2.2 Angstrom resolution. The enzyme was crystallized in space group P2(1) with four molecules in the asymmetric unit (V-m congruent to 2.6 Angstrom/Da). The overall fold consists of two domains of beta-barrel structures typical of the chymotrypsin family of serine proteinases. In general, the substrate binding sites, S4 to S3', are more polar than comparable sites in the related proteinase, human leukocyte elastase. The experimentally observed preference of PR3 for small aliphatic residues at the P1 position of a substrate is explained by the Val to Ile substitution at position 190 when compared to the elastase structure. The substitution of Ala by Asp at position 213 at the back of S1 should not affect its specificity greatly, as the Asp side-chain points back into the interior of the protein. The PR3 structure includes a disaccharide unit (N-linked 2-acetamido-2-deoxy-beta-D-glucopyranose and 1,6-linked alpha-L-fucopyranose) covalently attached to Asn159. The linear antigenic sites of PR3 reported to react with Wegener's granulomatosis autoantibodies occur in regions of the three-dimensional structure that may implicate the inactive pro-form of the enzyme in the pathogenesis of the disease. (C) 1996 Academic Press Limited

L30 ANSWER 45 OF 63 SCISEARCH COPYRIGHT (c) 2006 The Thomson Corporation on STN
ACCESSION NUMBER: 1996:165553 SCISEARCH Full-text
THE GENUINE ARTICLE: TX554
TITLE: Large-scale purification and preliminary X-ray diffraction studies of human aspartylglucosaminidase
AUTHOR: Tikkanen R (Reprint); Rouvinen J; Torronen A; Kalkkinen N; Peltonen L
CORPORATE SOURCE: NATL PUBL HLTH INST, DEPT HUMAN MOLEC GENET, MANNERHEIMINTIE 166, SF-00300 HELSINKI, FINLAND (Reprint); UNIV JOENSUU, DEPT CHEM, SF-80101 JOENSUU, FINLAND; UNIV HELSINKI, INST BIOTECHNOL, HELSINKI, FINLAND
COUNTRY OF AUTHOR: FINLAND
SOURCE: PROTEINS-STRUCTURE FUNCTION AND GENETICS, (FEB 1996) Vol. 24, No. 2, pp. 253-258.
ISSN: 0887-3585.
PUBLISHER: WILEY-LISS, DIV JOHN WILEY & SONS INC 605 THIRD AVE, NEW YORK, NY 10158-0012.
DOCUMENT TYPE: Article; Journal
FILE SEGMENT: LIFE
LANGUAGE: English
REFERENCE COUNT: 20
ENTRY DATE: Entered STN: 1996
Last Updated on STN: 1996
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB Aspartylglucosaminidase (AGA) is a lysosomal asparaginase that takes part in the ordered degradation of glycoproteins and a deficiency of which results in a lysosomal accumulation disease aspartylglucosaminuria in human, The mature enzyme consists of 24-kDa and 17-kDa subunits, which are both heterogeneously glycosylated, Activation of the enzyme from a single precursor polypeptide into two subunits is accomplished in the endoplasmic reticulum (ER). The relative lack of this proteolytic capacity in several tested high-producing expression systems has complicated the production of active recombinant enzyme in high quantities, which would be an alternative for purification of this molecule for crystallization, Consequently, the AGA enzyme has to be purified directly from cellular or tissue sources for crystallographic analysis, Here we describe a large-scale purification method to produce milligram amounts of homogeneous AGA from human leukocytes. The purified AGA enzyme represents a heterogeneous pool of molecules not only due to glycosylation, but also heterogeneity at the polypeptide level, as demonstrated here, We were able to isolate a homogeneous polypeptide pool that was successfully crystallized and preliminary X-ray data collected from the crystals, The crystals diffract well to 2.0 Angstrom and are thus suitable for determination of the crystal structure of AGA. (C) 1996 Wiley-Liss, Inc.

L30 ANSWER 46 OF 63 SCISEARCH COPYRIGHT (c) 2006 The Thomson Corporation on STN DUPLICATE 11
ACCESSION NUMBER: 1996:872923 SCISEARCH Full-text

THE GENUINE ARTICLE: VW127
TITLE: Molecular basis for amyloidosis related to hereditary brain hemorrhage
AUTHOR: Abrahamson M (Reprint)
CORPORATE SOURCE: UNIV LUND HOSP, DEPT CLIN CHEM, INST LAB MED, S-22185 LUND, SWEDEN (Reprint)
COUNTRY OF AUTHOR: SWEDEN
SOURCE: SCANDINAVIAN JOURNAL OF CLINICAL & LABORATORY INVESTIGATION, (1996) Vol. 56, Supp. [226], pp. 47-56. ISSN: 0036-5513.
PUBLISHER: SCANDINAVIAN UNIVERSITY PRESS, PO BOX 2959 TOYEN, JOURNAL DIVISION CUSTOMER SERVICE, N-0608 OSLO, NORWAY.
DOCUMENT TYPE: Article; Journal
FILE SEGMENT: LIFE; CLIN
LANGUAGE: English
REFERENCE COUNT: 44
ENTRY DATE: Entered STN: 1996
Last Updated on STN: 1996

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB The aim of the project has been to elucidate molecular events leading to amyloidosis in Hereditary Cystatin C Amyloid Angiopathy (HCCAA) patients, to enable simple diagnosis of the disease and with the ultimate goal to understand the amyloid formation process in detail, in order to develop inhibitors to the process. At the DNA level, a point mutation segregating with HCCAA was identified in the cystatin C gene on chromosome 20, after basic characterization of cDNA and gene for the wildtype protein. The mutation results in the amino acid substitution Leu-68-Gln (L68Q) and abolishes a recognition site for Alu I. This information was used to design a PCR based assay for simple and rapid mutation detection in DNA from blood samples to allow routine diagnosis of HCCAA. Studies at the protein level, allowed through E. coil expression of wildtype and L68Q mutated cystatin C genes, revealed that both protein variants effectively inhibit the cysteine proteinase cathepsin B (equilibrium constants for dissociation: 0.4 and 0.3 nM, respectively), but differ considerably in their tendency to dimerize and form aggregates. The initial dimerization of L68Q-cystatin C results in complete loss of biological activity and is highly temperature-dependent, with a rise in incubation temperature from 37 to 40 degrees C resulting in a 150% increase in dimerization rate. This result might be of clinical relevance, since medical intervention to abort febrile periods of carriers of the disease trait may reduce the in vivo formation of L68Q-cystatin C aggregates. The three-dimensional structure of normal cystatin C, crystallized in a complex with cathepsin B, was elucidated by X-ray analysis and subsequent refinement of the structure to 3.0 Angstrom resolution. Besides pinpointing the cystatin C structures resulting in efficient target enzyme inhibition, the results demonstrated that the Leu-68 residue is buried in the hydrophobic core of the protein. Studies of the three-dimensional solution structure of wildtype cystatin C by NMR spectroscopy revealed that cystatin C dimers can be formed as a result of slight, localized structural changes under conditions preceding complete defolding and denaturation of the protein. Dimers of L68Q-cystatin C are likely similar but are formed at temperatures nearly 30 degrees C lower than needed for the wildtype protein, indicating that the Leu-68-Gln substitution lowers the transition temperature for unfolding. Thus, the results presented suggest that cystatin C provides a system where decreased stability of a mutant protein correlates with its amyloidogenic nature. The NMR results furthermore imply that the hydrophobic proteinase-binding region of cystatin C is directly involved in dimer formation and that compounds designed to interact with this region could serve as inhibitors to the dimerization, and likely also the subsequent amyloid formation process, of cystatin C in HCCAA patients.

L30 ANSWER 47 OF 63 MEDLINE on STN
ACCESSION NUMBER: 97136130 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 8981667
TITLE: Molecular basis for amyloidosis related to hereditary brain hemorrhage.
AUTHOR: Abrahamson M
CORPORATE SOURCE: Department of Clinical Chemistry, University of Lund, University Hospital, Sweden.
SOURCE: Scandinavian journal of clinical and laboratory investigation. Supplementum, (1996) 226 47-56. Ref: 44
Journal code: 2984789R. ISSN: 0085-591X.
PUB. COUNTRY: Norway
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

General Review; (REVIEW)
(REVIEW, TUTORIAL)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199703
ENTRY DATE: Entered STN: 19970327
Last Updated on STN: 19970327
Entered Medline: 19970318

AB The aim of the project has been to elucidate molecular events leading to amyloidosis in Hereditary Cystatin C Amyloid Angiopathy (HCCAA) patients, to enable simple diagnosis of the disease and with the ultimate goal to understand the amyloid formation process in detail, in order to develop inhibitors to the process. At the DNA level, a point mutation segregating with HCCAA was identified in the cystatin C gene on chromosome 20, after basic characterization of cDNA and gene for the wildtype protein. The mutation results in the amino acid substitution Leu-68-Gin (L68Q) and abolishes a recognition site for Alu I. This information was used to design a PCR based assay for simple and rapid mutation detection in DNA from blood samples to allow routine diagnosis of HCCAA. Studies at the protein level, allowed through E. coli expression of wildtype and L68Q mutated cystatin C genes, revealed that both protein variants effectively inhibit the cysteine proteinase cathepsin B (equilibrium constants for dissociation: 0.4 and 0.3 nM, respectively), but differ considerably in their tendency to dimerize and form aggregates. The initial dimerization of L68Q-cystatin C results in complete loss of biological activity and is highly temperature-dependent, with a rise in incubation temperature from 37 to 40 degrees C resulting in a 150% increase in dimerization rate. This result might be of clinical relevance, since medical intervention to abort febrile periods of carriers of the disease trait may reduce the in vivo formation of L68Q-cystatin C aggregates. The three-dimensional structure of normal cystatin C, crystallized in a complex with cathepsin B, was elucidated by X-ray analysis and subsequent refinement of the structure to 3.0 A resolution. Besides pinpointing the cystatin C structures resulting in efficient target enzyme inhibition, the results demonstrated that the Leu-68 residue is buried in the hydrophobic core of the protein. Studies of the three-dimensional solution structure of wildtype cystatin C by NMR spectroscopy revealed that cystatin C dimers can be formed as a result of slight, localized structural changes under conditions preceding complete defolding and denaturation of the protein. Dimers of L68Q-cystatin C are likely similar but are formed at temperatures nearly 30 degrees C lower than needed for the wildtype protein, indicating that the Leu-68-Gln substitution lowers the transition temperature for unfolding. Thus, the results presented suggest that cystatin C provides a system where decreased stability of a mutant protein correlates with its amyloidogenic nature. The NMR results furthermore imply that the hydrophobic proteinase-binding region of cystatin C is directly involved in dimer formation and that compounds designed to interact with this region could serve as inhibitors to the dimerization, and likely also the subsequent amyloid formation process, of cystatin C in HCCAA patients.

L30 ANSWER 48 OF 63 MEDLINE on STN DUPLICATE 12
ACCESSION NUMBER: 95197558 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 7890671
TITLE: Crystal structures of recombinant rat cathepsin B and a cathepsin B-inhibitor complex. Implications for structure-based inhibitor design.
COMMENT: Erratum in: J Biol Chem 1995 Nov 24;270(47):28494
AUTHOR: Jia Z; Hasnain S; Hirama T; Lee X; Mort J S; To R; Huber C P
CORPORATE SOURCE: Institute for Biological Sciences, National Research Council of Canada, Ottawa.
SOURCE: Journal of biological chemistry, (1995 Mar 10) 270 (10) 5527-33.
Journal code: 2985121R. ISSN: 0021-9258.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199504
ENTRY DATE: Entered STN: 19950427
Last Updated on STN: 20000303
Entered Medline: 19950414

AB The lysosomal cysteine proteinase cathepsin B (EC 3.4.22.1) plays an important role in protein catabolism and has also been implicated in various disease states. The crystal structures of two forms of native recombinant rat cathepsin B have been determined. The overall folding of rat cathepsin B was shown to be very similar to that of the human liver

enzyme. The structure of the native enzyme containing an underivatized active site cysteine (Cys29) showed the active enzyme conformation to be similar to that determined previously for the oxidized form. In a second structure Cys29 was derivatized with the reversible blocking reagent pyridyl disulfide. In this structure large side chain conformational changes were observed for the two key catalytic residues Cys29 and His199, demonstrating the potential flexibility of these side chains. In addition the structure of the complex between rat cathepsin B and the inhibitor benzyloxycarbonyl-Arg- Ser(O-Bzl) chloromethylketone was determined. The complex structure showed that very little conformational change occurs in the enzyme upon inhibitor binding. It also allowed visualization of the interaction between the enzyme and inhibitor. In particular the interaction between Glu245 and the P2 Arg residue was clearly demonstrated, and it was found that the benzyl group of the P1 substrate residue occupies a large hydrophobic pocket thought to represent the S'1 subsite. This may have important implications for structure-based design of cathepsin B inhibitors.

L30 ANSWER 49 OF 63 MEDLINE on STN DUPLICATE 13
ACCESSION NUMBER: 95234708 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 7718586
TITLE: Crystal structure of cathepsin B inhibited with CA030 at 2.0-A resolution: A basis for the design of specific epoxysuccinyl inhibitors.
AUTHOR: Turk D; Podobnik M; Popovic T; Katunuma N; Bode W; Huber R; Turk V
CORPORATE SOURCE: Department of Biochemistry and Molecular Biology, Jozef Stefan Institute, Ljubljana, Slovenia.
SOURCE: Biochemistry, (1995 Apr 11) 34 (14) 4791-7.
Journal code: 0370623. ISSN: 0006-2960.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199505
ENTRY DATE: Entered STN: 19950605
Last Updated on STN: 19950605
Entered Medline: 19950523

AB Crystals of cysteine protease human cathepsin B inhibited with CA030 (ethyl ester of epoxysuccinyl-Ile-Pro-OH) [Murata, M., et al. (1991) FEBS Lett. 280, 307-310; Towatari, T., et al. (1991) FEBS Lett. 280, 311-315] were isomorphous to a previous published structure of cathepsin B [Musil, D., et al. (1991) EMBO J. 10, 2321-2330]. The crystal structure of the complex was refined at 2.0-A resolution to an R-value of 0.194. CA030 is well-defined in the electron density. The Ile-Pro-OH part of CA030 mimics a substrate P1' and P2' residues. The structure thus reveals for the first time a substratelike interaction in the S1' and S2' sites of a papain-like cysteine protease. The CA030 ethyl ester group occupies the S2 site. The structure confirms the role of residues His 110 and His 111 as the receptors of a peptidic substrate C-terminal carboxylic group. The structure suggests that an epoxysuccinyl fragment can be used to extend binding into primed and nonprimed substrate binding sites of a papain-like cysteine protease.

L30 ANSWER 50 OF 63 SCISEARCH COPYRIGHT (c) 2006 The Thomson Corporation on STN
ACCESSION NUMBER: 1995:811567 SCISEARCH Full-text
THE GENUINE ARTICLE: TG820
TITLE: THE CRYSTAL-STRUCTURE OF A MAJOR SECRETED ASPARTIC PROTEINASE FROM CANDIDA-ALBICANS IN COMPLEXES WITH 2 INHIBITORS
AUTHOR: CUTFIELD S M (Reprint); DODSON E J; ANDERSON B F; MOODY P C E; MARSHALL C J; SULLIVAN P A; CUTFIELD J F
CORPORATE SOURCE: UNIV OTAGO, DEPT BIOCHEM, DUNEDIN, NEW ZEALAND; UNIV YORK, DEPT CHEM, YORK YO1 5DD, N YORKSHIRE, ENGLAND; MASSEY UNIV, DEPT CHEM & BIOCHEM, PALMERSTON NORTH, NEW ZEALAND
COUNTRY OF AUTHOR: NEW ZEALAND; ENGLAND
SOURCE: STRUCTURE, (15 NOV 1995) Vol. 3, No. 11, pp. 1261-1271.
ISSN: 0969-2126.
PUBLISHER: CURRENT BIOLOGY LTD, 34-42 CLEVELAND STREET, LONDON, ENGLAND W1P 6LB.
DOCUMENT TYPE: Article; Journal
FILE SEGMENT: LIFE
LANGUAGE: English
REFERENCE COUNT: 47

ENTRY DATE: Entered STN: 1995
Last Updated on STN: 1995
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB Background: Infections caused by Candida albicans, a common fungal pathogen of humans, are increasing in incidence, necessitating development of new therapeutic drugs. Secreted aspartic proteinase (SAP) activity is considered an important virulence factor in these infections and might offer a suitable target for drug design. Amongst the various SAP isozymes, the SAP2 gene product is the major form expressed in a number of C. albicans strains.
Results: The three-dimensional structures of Sap2 complexed with the tight-binding inhibitor A70450 (a synthetic hexapeptide analogue) and with the general aspartic proteinase inhibitor pepstatin A (a microbial natural product) have been determined to 2.1 Angstrom and 3.0 Angstrom resolution, respectively. Although the protein structure retains the main features of a typical aspartic proteinase, it also shows some significant differences, due mainly to several sequence insertions and deletions (as revealed by homology modelling), that alter the shape of the binding cleft. There is also considerable variation in the C-terminal structural domain.
Conclusions: The differences in side chains, and in the conformations adopted by the two inhibitors, particularly at their P4, P3 and P'2 positions (using standard notation for protease-inhibitor residues), allows the A70450 structure to complement, more accurately, that of the substrate-binding site of SAP2. Some differences in the binding clefts of other SAP isoenzymes may be deduced from the SAP2 structure.

L30 ANSWER 51 OF 63 SCISEARCH COPYRIGHT (c) 2006 The Thomson Corporation on STN
ACCESSION NUMBER: 1995:317437 SCISEARCH Full-text
THE GENUINE ARTICLE: QW981
TITLE: CRYSTAL-STRUCTURE OF HUMAN PEPSIN AND ITS COMPLEX WITH PEPSTATIN
AUTHOR: FUJINAGA M (Reprint); CHERNAIA M M; TARASOVA N I; MOSIMANN S C; JAMES M N G
CORPORATE SOURCE: UNIV ALBERTA, DEPT BIOCHEM, EDMONTON, AB T6G 2H7, CANADA; NCI, FREDERICK CANC RES & DEV CTR, ABL, BASIC RES PROGRAM, MOLEC ASPECTS DRUG DESIGN SECT, FREDERICK, MD 21702
COUNTRY OF AUTHOR: CANADA; USA
SOURCE: PROTEIN SCIENCE, (MAY 1995) Vol. 4, No. 5, pp. 960-972. ISSN: 0961-8368.
PUBLISHER: CAMBRIDGE UNIV PRESS, 40 WEST 20TH STREET, NEW YORK, NY 10011-4211.
DOCUMENT TYPE: Article; Journal
FILE SEGMENT: LIFE
LANGUAGE: English
REFERENCE COUNT: 54
ENTRY DATE: Entered STN: 1995
Last Updated on STN: 1995
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB The three-dimensional crystal structure of human pepsin and that of its complex with pepstatin have been solved by X-ray crystallographic methods. The native pepsin structure has been refined with data collected to 2.2 Angstrom resolution to an R-factor of 19.7%. The pepsin:pepstatin structure has been refined with data to 2.0 Angstrom resolution to an R-factor of 18.5%. The hydrogen bonding interactions and the conformation adopted by pepstatin are very similar to those found in complexes of pepstatin with other aspartic proteinases. The enzyme undergoes a conformational change upon inhibitor binding to enclose the inhibitor more tightly. The analysis of the binding sites indicates that they form an extended tube without distinct binding pockets. By comparing the residues on the binding surface with those of the other human aspartic proteinases, it has been possible to rationalize some of the experimental data concerning the different specificities. At the S1 site, valine at position 120 in renin instead of isoleucine, as in the other enzymes, allows for binding of larger hydrophobic residues. The possibility of multiple conformations for the P2 residue makes the analysis of the S2 site difficult. However, it is possible to see that the specific interactions that renin makes with histidine at P2 would not be possible in the case of the other enzymes. At the S3 site, the smaller volume that is accessible in pepsin compared to the other enzymes is consistent with its preference for smaller residues at the P3 position.

L30 ANSWER 52 OF 63 MEDLINE on STN

ACCESSION NUMBER: 96073632 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 8540315
TITLE: Comparisons of the three-dimensional structures, specificities and glycosylation of renins, yeast proteinase A and cathepsin D.
AUTHOR: Aguilar C F; Dhanaraj V; Guruprasad K; Dealwis C; Badasso M; Cooper J B; Wood S P; Blundell T L
CORPORATE SOURCE: Department of Crystallography, Birkbeck College, London, UK.
SOURCE: Advances in experimental medicine and biology, (1995) 362 155-66.
Journal code: 0121103. ISSN: 0065-2598.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199602
ENTRY DATE: Entered STN: 19960221
Last Updated on STN: 20000303
Entered Medline: 19960206

AB The crystal structures of complexes of the aspartic proteinases, human and mouse renins, yeast proteinase A and cathepsin D, with peptide analogue inhibitors are compared. Differences occur in the relative positions of the domain comprising residues 190-302 (pepsin numbering) compared to the remaining structure and in the nature and position of the irregular regions joining the beta-strands and alpha-helices. The first three of the five residues of the oligosaccharide structures attached to Asn 67 of yeast proteinase and cathepsin D cover the same region of the protein surface. All enzymes have an unusual, proline-rich region (292-297) which acts as a second flap (in addition to that involving residues 72-81). This covers the active site cleft, but can be very close to the substrate/inhibitor at P3' and P4' only in the renins.

L30 ANSWER 53 OF 63 SCISEARCH COPYRIGHT (c) 2006 The Thomson Corporation on STN
ACCESSION NUMBER: 1995:59328 SCISEARCH Full-text
THE GENUINE ARTICLE: QB227
TITLE: NONPEPTIDIC INHIBITORS OF HUMAN-LEUKOCYTE ELASTASE .5. DESIGN, SYNTHESIS, AND X-RAY CRYSTALLOGRAPHY OF A SERIES OF ORALLY-ACTIVE 5-AMINOPYRIMIDIN-6-ONE-CONTAINING TRIFLUOROMETHYL KETONES
AUTHOR: VEALE C A (Reprint); BERNSTEIN P R; BRYANT C; CECCARELLI C; DAMEWOOD J R; EARLEY R; FEENEY S W; GOMES B; KOSMIDER B J; STEELMAN G B; THOMAS R M; VACEK E P; WILLIAMS J C; WOLANIN D J; WOOLSON S
CORPORATE SOURCE: ZENECA PHARMACEUT, DEPT MED CHEM, 1800 CONCORD PIKE, WILMINGTON, DE 19897 (Reprint); ZENECA PHARMACEUT, DEPT DRUG DISPOSIT & METAB, WILMINGTON, DE 19897; ZENECA PHARMACEUT, DEPT PHARMACOL, WILMINGTON, DE 19897
COUNTRY OF AUTHOR: USA
SOURCE: JOURNAL OF MEDICINAL CHEMISTRY, (6 JAN 1995) Vol. 38, No. 1, pp. 98-108.
ISSN: 0022-2623.
PUBLISHER: AMER CHEMICAL SOC, PO BOX 57136, WASHINGTON, DC 20037-0136
DOCUMENT TYPE: Article; Journal
FILE SEGMENT: LIFE
LANGUAGE: English
REFERENCE COUNT: 34
ENTRY DATE: Entered STN: 1995
Last Updated on STN: 1995
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB The effects of changes in Substitution in a series of 5-amino-2-pyrimidin-6-ones on both in vitro activity and oral activity in an acute hemorrhagic assay have been explored. These compounds contained either a trifluoromethyl ketone or a boronic acid moiety to bind covalently to the Ser-195 hydroxyl of human leukocyte elastase (HLE). Boronic acid-containing inhibitors were found to be more potent than the corresponding trifluoromethyl ketones in vitro but were less active upon oral administration. Compound 13b was found to offer the best combination of oral potency, duration of action, and enzyme selectivity and, as such, was selected for further biological testing. X- ray crystallography of a cocrystallized complex of

compound 19m and porcine pancreatic elastase demonstrated that the inhibitor is bound to the enzyme in a manner similar to that found previously for a closely related series of pyridone-containing inhibitors of HLE.

L30 ANSWER 54 OF 63 SCISEARCH COPYRIGHT (c) 2006 The Thomson Corporation on STN
ACCESSION NUMBER: 1995:59327 SCISEARCH Full-text
THE GENUINE ARTICLE: QB227
TITLE: NONPEPTIDIC INHIBITORS OF HUMAN-LEUKOCYTE ELASTASE .4. DESIGN, SYNTHESIS, AND IN-VITRO AND IN-VIVO ACTIVITY OF A SERIES OF BETA-CARBOLINONE-CONTAINING TRIFLUOROMETHYL KETONES
AUTHOR: VEALE C A (Reprint); DAMEWOOD J R; STEELMAN G B; BRYANT C; GOMES B; WILLIAMS J
CORPORATE SOURCE: ZENECA PHARMACEUT, DEPT MED CHEM, PULM CHEM SECT, WILMINGTON, DE 19897 (Reprint); ZENECA PHARMACEUT, DEPT PHARMACOL, WILMINGTON, DE 19897
COUNTRY OF AUTHOR: USA
SOURCE: JOURNAL OF MEDICINAL CHEMISTRY, (6 JAN 1995) Vol. 38, No. 1, pp. 86-97.
ISSN: 0022-2623.
PUBLISHER: AMER CHEMICAL SOC, PO BOX 57136, WASHINGTON, DC 20037-0136
DOCUMENT TYPE: Article; Journal
FILE SEGMENT: LIFE
LANGUAGE: English
REFERENCE COUNT: 46
ENTRY DATE: Entered STN: 1995
Last Updated on STN: 1995
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB A novel series of human leukocyte elastase (HLE) inhibitors containing the beta-carbolinone ring system are reported. The design of these trifluoromethyl ketone-based inhibitors used a combination of structural information obtained from X-ray crystallography and molecular modeling investigations. The beta-carbolinone ring in these compounds serves as a highly efficient peptidiomimetic for the P-2-P-3 region of peptidyl trifluoromethyl ketone inhibitors of HLE. Several of the beta-carbolinones exhibit significant in vitro potency, with K-i values in the nanomolar recognition of these inhibitors by HLE have been obtained and are discussed. This series of compounds are found to have excellent selectivity for HLE over a number of other proteolytic enzymes, including closely related enzymes such as porcine pancreatic elastase.

L30 ANSWER 55 OF 63 SCISEARCH COPYRIGHT (c) 2006 The Thomson Corporation on STN
ACCESSION NUMBER: 1994:634454 SCISEARCH Full-text
THE GENUINE ARTICLE: PJ408
TITLE: COMPARATIVE MODELING OF BARLEY-GRAIN ASPARTIC PROTEINASE - A STRUCTURAL RATIONALE FOR OBSERVED HYDROLYTIC SPECIFICITY
AUTHOR: GURUPRASAD K (Reprint); TORMAKANGAS K; KERVINEN J; BLUNDELL T L
CORPORATE SOURCE: UNIV LONDON BIRKBECK COLL, DEPT CRYSTALLOG, MOLEC BIOL LAB, LONDON WC1E 7HX, ENGLAND; UNIV HELSINKI, INST BIOTECHNOL, SF-00014 HELSINKI, FINLAND
COUNTRY OF AUTHOR: ENGLAND; FINLAND
SOURCE: FEBS LETTERS, (26 SEP 1994) Vol. 352, No. 2, pp. 131-136.
ISSN: 0014-5793.
PUBLISHER: ELSEVIER SCIENCE BV, PO BOX 211, 1000 AE AMSTERDAM, NETHERLANDS.
DOCUMENT TYPE: Article; Journal
FILE SEGMENT: LIFE
LANGUAGE: English
REFERENCE COUNT: 45
ENTRY DATE: Entered STN: 1994
Last Updated on STN: 1994
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB A model of the barley-grain aspartic proteinase (HvAP; Hordeum vulgare aspartic proteinase) has been constructed using the rule-based comparative modelling approach encoded in the COMPOSER suite of computer programs. The model was based on the high resolution crystal structures of six highly homologous aspartic

proteinases. Results suggest that the overall three-dimensional structure of HvAP (excluding the plant-specific insert; 104 residues in HvAP) is closer to human cathepsin D than other aspartic proteinases of known three-dimensional structure. Comparisons of the complexes with the substrate modelled in the active site of HvAP with those of the same substrate modelled in the active site of other aspartic proteinases of known three-dimensional structure and specificity, define residues that may influence hydrolytic specificity of the barley enzyme. We have identified residues in the S-4 (Ala(12)), S-3 (Gln(13), Thr(111)), S-2 (Ala(222), Thr(287), Met(289)), S-1' and S-3' (Ile(291)), S-2' and S-3' (Gln(74)), S-2' (Arg(295)), and S-3' (Pro(292)) pockets, that may account for the observed trends in the kinetic behaviour and specificity when compared to other aspartic proteinases. The plant-specific inserted sequence, which may play a role in the transport of HvAP to plant vacuoles (lysosomes), is similar to the saposins and is predicted to be a mixed alpha-helical and beta-strand domain.

L30 ANSWER 56 OF 63 MEDLINE on STN
ACCESSION NUMBER: 93342076 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 8393577
TITLE: Crystal structures of native and inhibited forms of human cathepsin D: implications for lysosomal targeting and drug design.
AUTHOR: Baldwin E T; Bhat T N; Gulnik S; Hosur M V; Sowder R C 2nd; Cachau R E; Collins J; Silva A M; Erickson J W
CORPORATE SOURCE: Structural Biochemistry Program, Program Resources Inc./DynCorp, National Cancer Institute-Frederick Cancer Research and Development Center, MD 21702.
CONTRACT NUMBER: N01-CO-74102 (NCI)
SOURCE: Proceedings of the National Academy of Sciences of the United States of America, (1993 Jul 15) 90 (14) 6796-800. Journal code: 7505876. ISSN: 0027-8424.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199308
ENTRY DATE: Entered STN: 19930917
Last Updated on STN: 20000303
Entered Medline: 19930830
AB Cathepsin D (EC 3.4.23.5) is a lysosomal protease suspected to play important roles in protein catabolism, antigen processing, degenerative diseases, and breast cancer progression. Determination of the crystal structures of cathepsin D and a complex with pepstatin at 2.5 A resolution provides insights into inhibitor binding and lysosomal targeting for this two-chain, N-glycosylated aspartic protease. Comparison with the structures of a complex of pepstatin bound to rhizopuspepsin and with a human renin-inhibitor complex revealed differences in subsite structures and inhibitor-enzyme interactions that are consistent with affinity differences and structure-activity relationships and suggest strategies for fine-tuning the specificity of cathepsin D inhibitors. Mutagenesis studies have identified a phosphotransferase recognition region that is required for oligosaccharide phosphorylation but is 32 A distant from the N-domain glycosylation site at Asn-70. Electron density for the crystal structure of cathepsin D indicated the presence of an N-linked oligosaccharide that extends from Asn-70 toward Lys-203, which is a key component of the phosphotransferase recognition region, and thus provides a structural explanation for how the phosphotransferase can recognize apparently distant sites on the protein surface.

L30 ANSWER 57 OF 63 MEDLINE on STN DUPLICATE 14
ACCESSION NUMBER: 93223670 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 8467789
TITLE: Two crystal structures for cathepsin D: the lysosomal targeting signal and active site.
AUTHOR: Metcalf P; Fusek M
CORPORATE SOURCE: European Molecular Biology Laboratory, Heidelberg, Germany.
SOURCE: EMBO journal, (1993 Apr) 12 (4) 1293-302. Journal code: 8208664. ISSN: 0261-4189.
PUB. COUNTRY: ENGLAND: United Kingdom
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199305

ENTRY DATE: Entered STN: 19930521
Last Updated on STN: 19930521
Entered Medline: 19930513

AB Two crystal structures are described for the lysosomal aspartic protease cathepsin D (EC 3.4.23.5). The molecular replacement method was used with X-ray diffraction data to 3 A resolution to produce structures for human spleen cathepsin D and for bovine liver cathepsin D complexed with the 6-peptide inhibitor pepstatin A. The lysosomal targeting region of cathepsin D defined by previous expression studies [Barnaski et al. (1990) Cell, 63, 281-219] is located in well defined electron density on the surface of the molecules. This region includes the putative binding site of the cis-Golgi phosphotransferase which is responsible for the initial sorting step for soluble proteins destined for lysosomes by phosphorylating the carbohydrates on these molecules. Carbohydrate density is visible at both expected positions on the cathepsin D molecules and, at the best defined position, four sugar residues extend towards the lysosomal targeting region. The active site of the protease and the active site cleft substrate binding subsites are described using the pepstatin inhibited structure. The model geometry for human cathepsin D has rms deviations from ideal of bonds and angles of 0.013 A and 3.2 degrees respectively. For bovine cathepsin D the corresponding figures are 0.014 A and 3.3 degrees. The crystallographic residuals (R factors) are 16.1% and 15.8% for the human and inhibited bovine cathepsin D models respectively. The free R factors, calculated with 10% of the data reserved for testing the models and not used for refinement, are 25.1% and 24.1% respectively.

L30 ANSWER 58 OF 63 SCISEARCH COPYRIGHT (c) 2006 The Thomson Corporation on STN
ACCESSION NUMBER: 1992:133658 SCISEARCH Full-text
THE GENUINE ARTICLE: HF639
TITLE: DESIGN, SYNTHESIS, AND KINETIC EVALUATION OF A UNIQUE CLASS OF ELASTASE INHIBITORS, THE PEPTIDYL ALPHA-KETOBENZOXAZOLES, AND THE X-RAY CRYSTAL-STRUCTURE OF THE COVALENT COMPLEX BETWEEN PORCINE PANCREATIC ELASTASE AND AC-ALA-PRO-VAL-2-BENZOXAZOLE
AUTHOR: EDWARDS P D (Reprint); MEYER E F; VIJAYALAKSHMI J; TUTHILL P A; ANDISIK D A; GOMES B; STRIMPLER A
CORPORATE SOURCE: ICI AMER INC, PHARMACEUT GRP, WILMINGTON, DE 19897 (Reprint); TEXAS A&M UNIV SYST, DEPT BIOCHEM & BIOPHYS, COLLEGE STN, TX 77843
COUNTRY OF AUTHOR: USA
SOURCE: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, (26 FEB 1992) Vol. 114, No. 5, pp. 1854-1863.
ISSN: 0002-7863.
PUBLISHER: AMER CHEMICAL SOC, 1155 16TH ST, NW, WASHINGTON, DC 20036.
DOCUMENT TYPE: Article; Journal
FILE SEGMENT: PHYS; LIFE
LANGUAGE: English
REFERENCE COUNT: 49
ENTRY DATE: Entered STN: 1994
Last Updated on STN: 1994
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB Peptidyl alpha-ketobenzoxazoles 1 and 2 are potent, competitive, reversible inhibitors of the serine proteinases HLE and PPE. These inhibitors were designed to inactivate the enzyme by interacting with both the serine hydroxyl group and the histidine imidazole ring of the catalytic triad. The X-ray crystal structure determination of 2 bound to PPE confirms the covalent attachment of the inhibitor's carbonyl carbon atom to the hydroxyl group of the active site Ser-195. The nitrogen atom of the benzoxazole ring participates in a hydrogen-bonding interaction with His-57. This is the first example of a reversible inhibitor designed to take advantage of the binding opportunities afforded by both the serine and the histidine of the catalytic triad in serine proteinases.

L30 ANSWER 59 OF 63 SCISEARCH COPYRIGHT (c) 2006 The Thomson Corporation on STN
ACCESSION NUMBER: 1992:220119 SCISEARCH Full-text
THE GENUINE ARTICLE: HK860
TITLE: EFFECT OF THE 7-AMINO SUBSTITUENT ON THE INHIBITORY POTENCY OF MECHANISM-BASED ISOCOUMARIN INHIBITORS FOR PORCINE PANCREATIC AND HUMAN NEUTROPHIL ELASTASES - A 1.85-A X-RAY STRUCTURE

OF THE COMPLEX BETWEEN PORCINE PANCREATIC ELASTASE AND 7-[(N-TOSYLPHENYLALANYL)AMINO]-4-CHLORO-3-METHOXYISOCOUMARIN

AUTHOR: HERNANDEZ M A (Reprint); POWERS J C; GLINSKI J; OLEKSYSZYN J; VIJAYALAKSHMI J; MEYER E F

CORPORATE SOURCE: GEORGIA INST TECHNOL, SCH CHEM & BIOCHEM, ATLANTA, GA 30332; TEXAS A&M UNIV SYST, DEPT BIOCHEM & BIOPHYS, COLLEGE STN, TX 77843

COUNTRY OF AUTHOR: USA

SOURCE: JOURNAL OF MEDICINAL CHEMISTRY, (20 MAR 1992) Vol. 35, No. 6, pp. 1121-1129.
ISSN: 0022-2623.

PUBLISHER: AMER CHEMICAL SOC, 1155 16TH ST, NW, WASHINGTON, DC 20036.

DOCUMENT TYPE: Article; Journal

FILE SEGMENT: LIFE

LANGUAGE: English

REFERENCE COUNT: 31

ENTRY DATE: Entered STN: 1994
Last Updated on STN: 1994

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB A series of new acyl, urea, and carbonate derivatives of 7-amino-4-chloro-3-methoxyisocoumarin were synthesized and evaluated as irreversible inhibitors of human neutrophil elastase (HNE) and porcine pancreatic elastase (PPE). Inhibition of HNE is directly related to the hydrophobicity of the substituent on the 7-amino group. The N-Tos-Phe derivative (19) is the best HNE inhibitor with a second-order rate constant k(obs)/[I] = 200 000 M-1 s-1. The closest analogue in this series, the 3,3-diphenylpropionyl derivative 5, had a k(obs)/[I] = 130 000 M-1 s-1 with HNE. In contrast to the Tos-Phe derivative 19, phenylacetyl derivative 2 and carbonates 22 and 25 gave extremely stable enzyme-inhibitor complexes with deacylation half-lives longer than 48 h with both elastases. N-Phenylurea derivative 25 was the best inhibitor for PPE with a second-order rate constant k(obs)/[I] = 7300 M-1 s-1. The crystal structure of a complex of PPE with N-tosyl-Phe derivative 19 was determined at 1.85-angstrom resolution and refined to a final R factor of 16.9%. The isocoumarin forms an acyl enzyme with Ser-195, while His-57 is near the inhibitor, but not covalently linked. The Tos-Phe makes a few hydrophobic contacts with the S' subsites of PPE, but appears to be interacting primarily with itself in the PPE structure. This region of HNE is more hydrophobic and modeling indicates that the inhibitor would probably make additional contacts with the enzyme.

L30 ANSWER 60 OF 63 EMBASE

ACCESSION NUMBER: 92264558 EMBASE Full-text

DOCUMENT NUMBER: 1992264558

TITLE: Inhibition of human serine proteases by substituted 2-azetidinones.

AUTHOR: Knight W.B.; Chabin R.; Green B.

CORPORATE SOURCE: Department of Enzymology, Building 80Y-150, Merck, Sharp/Dohme Research Lab., P.O. Box 2000,Rahway, NJ 07065, United States

SOURCE: Archives of Biochemistry and Biophysics, (1992) Vol. 296, No. 2, pp. 704-708.
ISSN: 0003-9861 CODEN: ABBIA4

COUNTRY: United States

DOCUMENT TYPE: Journal; Article

FILE SEGMENT: 029 Clinical Biochemistry

LANGUAGE: English

SUMMARY LANGUAGE: English

ENTRY DATE: Entered STN: 921004
Last Updated on STN: 921004

AB trans-4-Ethoxycarbonyl-3-ethyl-1-(4-nitrophenylsulfonyl)-azetidin-3-one described by Firestone et al. (1990, Tetrahedron 46, 2255) as an inhibitor of human leucocyte elastase (HLE) displayed potent, time-dependent inhibition of both HLE and human cathepsin G (Cat-G). The cis-isomer was 7- and 180-fold less active, respectively. The mechanism likely involves opening of the β- lactam ring by the active site serine to form an acyl-enzyme intermediate(s). This intermediate partitions with ratios of 4:1 between turnover of the inhibitor and formation of relatively stable enzyme-inhibitor complexes from both enzymes. The final HLE-inhibitor complex reactivated with a half-life of 48 h at 25°C and was 16-fold more stable than the Cat-G-inhibitor complex. The stability of the acyl-enzymes supports a 'double hit' chemical mechanism involving both serine acylation and alkylation

of the histidine. These observations suggest that β-lactams may be developed as a class of serine protease inhibitors.

L30 ANSWER 61 OF 63 MEDLINE on STN DUPLICATE 15
ACCESSION NUMBER: 91162567 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 2002469
TITLE: Renin inhibitors containing conformationally restricted P1-P1' dipeptide mimetics.
AUTHOR: Williams P D; Perlow D S; Payne L S; Holloway M K; Siegl P K; Schorn T W; Lynch R J; Doyle J J; Strouse J F; Vlasuk G P; +
CORPORATE SOURCE: Merck Sharp and Dohme Research Laboratories, West Point, Pennsylvania 19486.
SOURCE: Journal of medicinal chemistry, (1991 Mar) 34 (3) 887-900. Journal code: 9716531. ISSN: 0022-2623.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199104
ENTRY DATE: Entered STN: 19910505
Last Updated on STN: 19970203
Entered Medline: 19910417

AB A series of renin inhibitors containing lactam-bridged P1-P1' dipeptide mimetics based on the ACHPA (4(S)-amino-5-cyclohexyl-3(S)-hydroxypentanoic acid) design was studied. The inhibitors were obtained by aldol addition of various lactams with N alpha-Boc-L-cyclohexylalaninal, followed by Boc group removal and acylation with Boc-Phe-His. The aldol diastereomer having the S configuration at the two newly generated stereogenic centers gave optimal enzyme inhibition. Potency was further enhanced in the gamma-lactam ring series by substitution with small hydrophobic groups to mimic the P1' side chain of the renin substrate. Thus, 2(S)-[(Boc-L-phenylalanyl-L-histidyl)amino]-3-cyclohexyl-1(S)-hydroxyl-1 - (1,5,5-trimethyl-2-oxopyrrolidin-3(S)-yl)propane (34) has an IC50 of 1.3 nM in the human plasma renin assay. A variety of substituents on the lactam nitrogen are tolerated and can be used to vary the physical properties of the inhibitor. By using a model of the human renin active site, the conformation of 34 in the enzyme-inhibitor complex is proposed. This modeled conformation is very similar to the solid-state conformation of 2(S)-[(Boc-L-phenylalanyl-L- histidyl)amino]-3-cyclohexyl-1(S)-hydroxyl-1-(1-methyl-2-oxopyrrolidin- 3(S)-yl)propane (36), the structure of which was determined by single- crystal X-ray diffraction analysis. The most potent ACH-PA-lactam renin inhibitors show good selectivity when assayed against other types of aspartic proteinases. By varying the lactam ring substituents, potent and selective inhibitors of cathepsin D and cathepsin E can be obtained.

L30 ANSWER 62 OF 63 MEDLINE on STN DUPLICATE 16
ACCESSION NUMBER: 91012489 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 2120440
TITLE: Orally potent human renin inhibitors derived from angiotensinogen transition state: design, synthesis, and mode of interaction.
AUTHOR: Iizuka K; Kamijo T; Harada H; Akahane K; Kubota T; Umeyama H; Ishida T; Kiso Y
CORPORATE SOURCE: Central Research Laboratories, Kissei Pharmaceutical Company, Ltd., Nagano, Japan.
SOURCE: Journal of medicinal chemistry, (1990 Oct) 33 (10) 2707-14. Journal code: 9716531. ISSN: 0022-2623.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199011
ENTRY DATE: Entered STN: 19910117
Last Updated on STN: 19970203
Entered Medline: 19901120

AB A three-dimensional structure of the complex of human renin and the scissile site P4 Pro to P1' Val of angiotensinogen was deduced in order to design potent human renin inhibitors rationally. On the basis of this structure, an orally potent human renin inhibitor (1a) was designed from the angiotensinogen transition state and synthesized. The inhibitor 1a contains a (2R)-3-(morpholinocarbonyl)-2-(1-naphthylmethyl)propionyl residue (P4-P3) with a retro-inverso amide bond, L-histidine, and a novel amino acid, (2R,3S)-3-amino-4-

cyclohexyl-2-hydroxybutyric acid, named cyclohexylnorstatine (2a). The optically pure cyclohexylnorstatine was efficiently prepared from Boc-L-cyclohexylalaninol (3), and the stereochemistry of 1a was established by X-ray crystal analysis. The analyses of interaction between 1a and human renin using modeling techniques indicated that (1) the cyclohexyl group of P1 and the naphthyl group of P3 were accommodated in large hydrophobic subsites S1 and S3, respectively; (2) the imidazole of P2 His was hydrogen bonded to the side chain OH of Ser-233 to contribute to the selectivity of renin inhibition; (3) cyclohexylnorstatine isopropyl ester residue was accommodated in S1-S1'. The importance of the stereochemistry in the potent and specific inhibitor was clearly shown. Oral administration to monkeys of this inhibitor resulted in a drop of 10-20 mmHg in mean blood pressure and a reduction of plasma renin activity for a 5-h period.

L30 ANSWER 63 OF 63 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:569990 CAPLUS Full-text
DOCUMENT NUMBER: 111:169990
TITLE: X-ray studies of aspartic proteinase-statine inhibitor complexes
AUTHOR(S): Cooper, J. B.; Foundling, S. I.; Blundell, T. L.; Boger, J.; Jupp, R. A.; Kay, J.
CORPORATE SOURCE: Dep. Crystallogr., Birkbeck Coll., London, WC1E 7HX, UK
SOURCE: Biochemistry (1989), 28(21), 8596-603
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The conformation of a statine-containing renin inhibitor (L 363564) complexed with the aspartic proteinase from the fungus, Endothia parasitica (EC 3.4.23.6), was determined by x-ray diffraction at 2.2-Å resolution (R = 0.17). The structure of the complex at high resolution was described and compared with a 3.0-Å resolution anal. of a bound inhibitor, L 364099, containing a cyclohexylalanine analog of statine. The inhibitors bound in extended conformations in the long active-site cleft, and the OH group of the transition-state analog, statine, interacted strongly with the catalytic aspartates via H bonds to the essential carboxyl groups. This work provides a detailed structural anal. of the role of statine in peptide inhibitors. It shows conclusively that statine should be considered a dipeptide analog (occupying residues P1 to P1') despite lacking the equivalent of a P1' side-chain, although other inhibitor residues (especially P2) may compensate by interacting at the unoccupied S1' specificity subsite.

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=> d his

(FILE 'HOME' ENTERED AT 11:37:39 ON 26 JAN 2006)

FILE 'REGISTRY' ENTERED AT 11:37:55 ON 26 JAN 2006

FILE 'MEDLINE, CAPLUS, SCISEARCH, LIFESCI, BIOSIS, EMBASE' ENTERED AT 11:39:00 ON 26 JAN 2006

L1	131	FILE MEDLINE
L2	103	FILE CAPLUS
L3	119	FILE SCISEARCH
L4	11	FILE LIFESCI
L5	59	FILE BIOSIS
L6	79	FILE EMBASE
	TOTAL FOR ALL FILES	
L7	502	S (CATHEPSIN OR SCATS) AND CRYSTAL? AND X-RAY
L8	90	FILE MEDLINE
L9	53	FILE CAPLUS
L10	65	FILE SCISEARCH
L11	5	FILE LIFESCI
L12	31	FILE BIOSIS
L13	47	FILE EMBASE
	TOTAL FOR ALL FILES	
L14	291	S L7 AND HUMAN
L15	34	FILE MEDLINE
L16	27	FILE CAPLUS
L17	35	FILE SCISEARCH
L18	1	FILE LIFESCI

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L19          13 FILE BIOSIS
L20          19 FILE EMBASE
     TOTAL FOR ALL FILES
L21         129 S L14 AND (LIGAND OR COMPLEX?)
L22          79 DUP REM L21 (50 DUPLICATES REMOVED)
L23          31 FILE MEDLINE
L24          17 FILE CAPLUS
L25          32 FILE SCISEARCH
L26           1 FILE LIFESCI
L27          12 FILE BIOSIS
L28          15 FILE EMBASE
     TOTAL FOR ALL FILES
L29         108 S L21 NOT 2004-2006/PY
L30          63 DUP REM L29 (45 DUPLICATES REMOVED)

=> s (cathepsin S or cats) and crystal? and x-ray
L31          49 FILE MEDLINE
L32          29 FILE CAPLUS
L33          18 FILE SCISEARCH
L34           4 FILE LIFESCI
L35          15 FILE BIOSIS
L36          10 FILE EMBASE

TOTAL FOR ALL FILES
L37         125 (CATHEPSIN S OR CATS) AND CRYSTAL? AND X-RAY

=> s l37 and human
L38          19 FILE MEDLINE
L39          12 FILE CAPLUS
L40           5 FILE SCISEARCH
L41           2 FILE LIFESCI
L42           5 FILE BIOSIS
L43           8 FILE EMBASE

TOTAL FOR ALL FILES
L44          51 L37 AND HUMAN

=> s l37 not 2004-2006/py
L45          48 FILE MEDLINE
L46          25 FILE CAPLUS
L47          16 FILE SCISEARCH
L48           4 FILE LIFESCI
L49          15 FILE BIOSIS
L50           9 FILE EMBASE

TOTAL FOR ALL FILES
L51         117 L37 NOT 2004-2006/PY

=> dup rem l51
PROCESSING COMPLETED FOR L51
L52          81 DUP REM L51 (36 DUPLICATES REMOVED)

=> s l51 and (ligand or complex)
L53          13 FILE MEDLINE
L54           4 FILE CAPLUS
L55           1 FILE SCISEARCH
L56           0 FILE LIFESCI
L57           2 FILE BIOSIS
L58           4 FILE EMBASE

TOTAL FOR ALL FILES
L59          24 L51 AND (LIGAND OR COMPLEX)

=> dup rem l59
PROCESSING COMPLETED FOR L59
L60          22 DUP REM L59 (2 DUPLICATES REMOVED)

=> d ibib abs 1-22

L60  ANSWER 1 OF 22  CAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:        2003:590728  CAPLUS Full-text
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DOCUMENT NUMBER: 139:145839
TITLE: Crystal structure of a human cathepsin S mutant, apparatus displaying a three-dimensional representation of the cathepsin S and applications to drug screening and design
INVENTOR(S): Lamers, Marieke B.; Williams, David H.; Turkenburg, Johan P.; Hubbard, Roderick E.
PATENT ASSIGNEE(S): Medivir Uk Ltd., UK
SOURCE: U.S. Pat. Appl. Publ., 59 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003143714	A1	20030731	US 2002-273577	20021018
PRIORITY APPLN. INFO.:			US 2001-330191P P	20011019

AB The invention relates to the X-ray crystal structure of a human cathepsin S mutant. The invention further relates to an apparatus programmed with one or more of the structure coordinates of the cathepsin S binding pockets, wherein said apparatus is capable of displaying a three-dimensional representation of that binding pocket. The invention also relates to methods of using the structure coordinates of a mutant cathepsin S to screen and design compds. that bind to the active site and accessory binding site of cathepsin S.

L60 ANSWER 2 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:952922 CAPLUS Full-text
DOCUMENT NUMBER: 140:141541
TITLE: Peptide Ketobenzoxazole Inhibitors Bound to Cathepsin K
AUTHOR(S): McGrath, Mary E.; Sprengeler, Paul A.; Hill, Craig M.; Martichonok, Valeri; Cheung, Harry; Somoza, John R.; Palmer, James T.; Janc, James W.
CORPORATE SOURCE: Celera, South San Francisco, CA, 94080, USA
SOURCE: Biochemistry (2003), 42(51), 15018-15028
CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:141541
AB Potent inhibitors of human cysteine proteases of the papain family have been made and assayed vs. a number of relevant family members. The authors describe the synthesis of peptide α-ketoheterocyclic inhibitors that occupy binding subsites S1'-S3 of the cysteine protease substrate recognition cleft and that form a reversible covalent bond with the Cys-25 nucleophile. X-ray crystal structures of cathepsin K both unbound and complexed with inhibitors provide detailed information on protease/inhibitor interactions and suggestions for the design of tight-binding, selective mols.
REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L60 ANSWER 3 OF 22 MEDLINE on STN
ACCESSION NUMBER: 2003520643 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 14581558
TITLE: Structures of host range-controlling regions of the capsids of canine and feline parvoviruses and mutants.
AUTHOR: Govindasamy Lakshmanan; Hueffer Karsten; Parrish Colin R; Agbandje-McKenna Mavis
CORPORATE SOURCE: Department of Biochemistry and Molecular Biology, Center for Structural Biology, College of Medicine, University of Florida, Gainesville, Florida 32610, USA.
CONTRACT NUMBER: AI33468 (NIAID)
SOURCE: Journal of virology, (2003 Nov) 77 (22) 12211-21.
Journal code: 0113724. ISSN: 0022-538X.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200311

ENTRY DATE: Entered STN: 20031106
Last Updated on STN: 20031219
Entered Medline: 20031125

AB Canine parvovirus (CPV) and feline panleukopenia virus (FPV) differ in their ability to infect dogs and dog cells. Canine cell infection is a specific property of CPV and depends on the ability of the virus to bind the canine transferrin receptor (TfR), as well as other unidentified factors. Three regions in the capsid structure, located around VP2 residues 93, 300, and 323, can all influence canine TfR binding and canine cell infection. These regions were compared in the CPV and FPV capsid structures that have been determined, as well as in two new structures of CPV capsids that contain substitutions of the VP2 Asn-93 to Asp and Arg, respectively. The new structures, determined by X-ray crystallography to 3.2 and 3.3 A resolutions, respectively, clearly showed differences in the interactions of residue 93 with an adjacent loop on the capsid surface. Each of the three regions show small differences in structure, but each appears to be structurally independent of the others, and the changes likely act together to affect the ability of the capsid to bind the canine TfR and to infect canine cells. This emphasizes the complex nature of capsid alterations that change the virus-cell interaction to allow infection of cells from different hosts.

L60 ANSWER 4 OF 22 MEDLINE on STN
ACCESSION NUMBER: 2003143398 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 12641451
TITLE: Specificity determinants of human cathepsin s revealed by crystal structures of complexes.
AUTHOR: Pauly Thomas A; Sulea Traian; Ammirati Mark; Sivaraman J; Danley Dennis E; Griffor Matthew C; Kamath Ajith V; Wang I-K; Laird Ellen R; Seddon Andrew P; Menard Robert; Cygler Miroslaw; Rath Virginia L
CORPORATE SOURCE: Exploratory Medicinal Sciences and Computational Chemistry, Groton Laboratories, Pfizer Global Research and Development, Eastern Point Road, Groton, Connecticut 06340, USA.
SOURCE: Biochemistry, (2003 Mar 25) 42 (11) 3203-13.
Journal code: 0370623. ISSN: 0006-2960.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
OTHER SOURCE: PDB-1NPZ; PDB-1NQC
ENTRY MONTH: 200304
ENTRY DATE: Entered STN: 20030328
Last Updated on STN: 20030418
Entered Medline: 20030417

AB Cathepsin S, a lysosomal cysteine protease of the papain superfamily, has been implicated in the preparation of MHC class II alphabeta-heterodimers for antigen presentation to CD4+ T lymphocytes and is considered a potential target for autoimmune-disease therapy. Selective inhibition of this enzyme may be therapeutically useful for attenuating the hyperimmune responses in a number of disorders. We determined the three-dimensional crystal structures of human cathepsin S in complex with potent covalent inhibitors, the aldehyde inhibitor 4-morpholinecarbonyl-Phe-(S-benzyl)Cys- Psi(CH=O), and the vinyl sulfone irreversible inhibitor 4-morpholinecarbonyl-Leu-Hph-Psi(CH=CH-SO(2)-phenyl) at resolutions of 1.8 and 2.0 A, respectively. In the structure of the cathepsin S-aldehyde complex, the tetrahedral thiohemiacetal adduct favors the S-configuration, in which the oxygen atom interacts with the imidazole group of the active site His164 rather than with the oxyanion hole. The present structures provide a detailed map of noncovalent intermolecular interactions established in the substrate-binding subsites S3 to S1' of cathepsin S. In the S2 pocket, which is the binding affinity hot spot of cathepsin S, the Phe211 side chain can assume two stable conformations that accommodate either the P2-Leu or a bulkier P2-Phe side chain. This structural plasticity of the S2 pocket in cathepsin S explains the selective inhibition of cathepsin S over cathepsin K afforded by inhibitors with the P2-Phe side chain. Comparison with the structures of cathepsins K, V, and L allows delineation of local intermolecular contacts that are unique to cathepsin S.

L60 ANSWER 5 OF 22 MEDLINE on STN DUPLICATE 1
ACCESSION NUMBER: 2003263873 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 12790167
TITLE: Analysis of feline urinary calculi and urethral plugs by infrared spectroscopy and scanning electron microscopy.

AUTHOR: Escolar E; Bellanato J
CORPORATE SOURCE: Departamento de Patologia Animal II, Hospital Clinico Veterinario, Universidad Complutense de Madrid, 28040 Madrid, Spain.
SOURCE: Veterinary record, (2003 May 17) 152 (20) 625-8. Journal code: 0031164. ISSN: 0042-4900.
PUB. COUNTRY: England: United Kingdom
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200308
ENTRY DATE: Entered STN: 20030608
Last Updated on STN: 20030805
Entered Medline: 20030804

AB The chemical constituents of 34 feline urinary calculi and five urethral plugs were analysed by infrared spectroscopy. The analysis revealed that 18 (52.9 per cent) of the calculi contained magnesium ammonium phosphate hexahydrate (struvite) as the major component; 10 (29.4 per cent) contained complex ammonium urates (three of them also containing calcium phosphate, mainly on the surface); three were composed of calcium phosphates and three were composed mainly of calcium oxalate mono and dihydrates. The urethral plugs were composed primarily of struvite, but also contained large amounts of organic matter. The examination of 16 selected samples by scanning electron microscopy and electron dispersive x-ray analysis revealed that their crystalline structures were similar to those of canine stones.

L60 ANSWER 6 OF 22 EMBASE COPYRIGHT (c) 2006 Elsevier B.V. All rights reserved on STN
ACCESSION NUMBER: 2003284758 EMBASE Full-text
TITLE: Drug-specific cyclodextrins: The future of rapid neuromuscular block reversal?.
AUTHOR: Zhang M.-Q.
CORPORATE SOURCE: M.-Q. Zhang, Shire BioChem Inc., 275 Armand-Frappier Blvd., Laval, Que. H7V 4A7, United Kingdom
SOURCE: Drugs of the Future, (1 Apr 2003) Vol. 28, No. 4, pp. 347-354.
Refs: 25
ISSN: 0377-8282 CODEN: DRFUD4
COUNTRY: Spain
DOCUMENT TYPE: Journal; General Review
FILE SEGMENT: 030 Pharmacology
037 Drug Literature Index
052 Toxicology
LANGUAGE: English
SUMMARY LANGUAGE: English
ENTRY DATE: Entered STN: 20030731
Last Updated on STN: 20030731

AB Chemical modification of γ-cyclodextrin afforded Org-25969 that has a cavity dimension capable of forming a binary host-guest complex with the steroidal neuromuscular blocker rocuronium bromide with high affinity. In this complex, rocuronium is encapsulated inside the cavity of Org-25969. As a consequence, the neuromuscular blocking activity of rocuronium can be reversed by Org-25969. The reversal produced by Org-25969 is more efficacious than the standard combination of acetylcholinesterase inhibitor and muscarinic receptor antagonist, e.g., neostigmine + atropine. Unlike neostigmine + atropine, Org-25969 does not interfere with the acetylcholine homeostasis. At the effective reversal dose (0.5 μmol/kg i.v.), Org-25969 produced negligible changes in hemodynamic parameters in anesthetized guinea pigs, cats and monkeys. Org-25969 is also effective in reversing profound block induced by 3 times the ED(90) of rocuronium in guinea pigs at a rate at least 3 times faster than neostigmine + atropine. Therefore, Org-25969 is also potentially useful for early or escape reversal of rocuronium, for instance, in a "cannot intubate, cannot ventilate" situation.

L60 ANSWER 7 OF 22 MEDLINE on STN DUPLICATE 2
ACCESSION NUMBER: 2002148581 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 11856830
TITLE: Structure of a Cys25-->Ser mutant of human cathepsin S.
AUTHOR: Turkenburg Johan P; Lamers Marieke B A C; Brzozowski A Marek; Wright Lisa M; Hubbard Roderick E; Sturt Simone L; Williams David H

CORPORATE SOURCE: York Structural Biology Laboratory, Chemistry Department, University of York, Heslington, York YO10 5DD, England.
SOURCE: Acta crystallographica. Section D, Biological crystallography, (2002 Mar) 58 (Pt 3) 451-5. Electronic Publication: 2002-02-21.
Journal code: 9305878. ISSN: 0907-4449.
PUB. COUNTRY: Denmark
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
OTHER SOURCE: PDB-1GLO
ENTRY MONTH: 200206
ENTRY DATE: Entered STN: 20020308
Last Updated on STN: 20020619
Entered Medline: 20020618

AB Cathepsin S (EC 3.4.22.27), a cysteine proteinase of the papain superfamily, plays a critical role in the generation of a major histocompatibility complex (MHC) class II restricted T-cell response by antigen-presenting cells. Therefore, selective inhibition of this enzyme may be useful in modulating class II restricted T-cell responses in immune-related disorders such as rheumatoid arthritis, multiple sclerosis and extrinsic asthma. The three-dimensional structure at 2.2 A resolution of the active-site Cys25-->Ser mutant presented here in an unliganded state provides further insight useful for the design of selective enzyme inhibitors.

L60 ANSWER 8 OF 22 EMBASE COPYRIGHT (c) 2006 Elsevier B.V. All rights reserved on STN
ACCESSION NUMBER: 2002345470 EMBASE Full-text
TITLE: Novel protease inhibitors.
AUTHOR: Norman P.
CORPORATE SOURCE: Dr. P. Norman, Norman Consulting, 18 Pink Lane, Burnham, Buckx, SL1 8JW, United Kingdom
SOURCE: Drug News and Perspectives, (2002) Vol. 15, No. 6, pp. 372-382.
ISSN: 0214-0934 CODEN: DNPEED
COUNTRY: Spain
DOCUMENT TYPE: Journal; Conference Article
FILE SEGMENT: 030 Pharmacology
037 Drug Literature Index
LANGUAGE: English
SUMMARY LANGUAGE: English
ENTRY DATE: Entered STN: 20021017
Last Updated on STN: 20021017

AB The Third RSC-SCI Symposium on Proteinase Inhibitor Design: Proteinase 2002, held May 13-14, 2002, in London, United Kingdom, drew an audience of about 140 scientists to the SCI's Belgrave Square headquarters to hear 17 speakers address various aspects of this theme. There was considerable emphasis placed upon the use of X-ray crystallography of enzyme-inhibitor complex as an integral tool in the design of improved protease inhibitors. This biennial meeting has established a reputation for being a key forum for the disclosure of new compounds, and this year's meeting was no exception, with much of the emphasis placed on novel inhibitors of either serine or cysteine proteases.

L60 ANSWER 9 OF 22 EMBASE COPYRIGHT (c) 2006 Elsevier B.V. All rights reserved on STN
ACCESSION NUMBER: 2002304948 EMBASE Full-text
TITLE: The cell biology of antigen presentation.
AUTHOR: Hudson A.W.; Ploegh H.L.
CORPORATE SOURCE: H.L. Ploegh, Department of Pathology, Harvard Medical School, 200 Longwood Avenue, Boston, MA 02115, United States. ploegh@hms.harvard.edu
SOURCE: Experimental Cell Research, (2002) Vol. 272, No. 1, pp. 1-7.
Refs: 33
ISSN: 0014-4827 CODEN: ECREAL
COUNTRY: United States
DOCUMENT TYPE: Journal; (Short Survey)
FILE SEGMENT: 026 Immunology, Serology and Transplantation
029 Clinical Biochemistry
LANGUAGE: English

ENTRY DATE: Entered STN: 20020913
Last Updated on STN: 20020913
DATA NOT AVAILABLE FOR THIS ACCESSION NUMBER

L60 ANSWER 10 OF 22 MEDLINE on STN
ACCESSION NUMBER: 2000481807 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 10957629
TITLE: Structures of feline immunodeficiency virus dUTP pyrophosphatase and its nucleotide complexes in three crystal forms.
AUTHOR: Prasad G S; Stura E A; Elder J H; Stout C D
CORPORATE SOURCE: Department of Molecular Biology, The Scripps Research Institute, La Jolla, CA 92037-1093, USA.. prasad@scripps.edu
CONTRACT NUMBER: AI25825 (NIAID)
GM48495 (NIGMS)
MH47680 (NIMH)
SOURCE: Acta crystallographica. Section D, Biological crystallography, (2000 Sep) 56 (Pt 9) 1100-9.
Journal code: 9305878. ISSN: 0907-4449.
PUB. COUNTRY: Denmark
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals; AIDS
OTHER SOURCE: PDB-1F7D; PDB-1F7K; PDB-1F7N; PDB-1F7O; PDB-1F7P; PDB-1F7Q; PDB-1F7R
ENTRY MONTH: 200010
ENTRY DATE: Entered STN: 20001019
Last Updated on STN: 20001019
Entered Medline: 20001010

AB dUTP pyrophosphatase (dUTPase) cleaves the alpha-beta phosphodiester of dUTP to form pyrophosphate and dUMP, preventing incorporation of uracil into DNA and providing the substrate for thymine synthesis. Seven crystal structures of feline immunodeficiency virus (FIV) dUTPase in three crystal forms have been determined, including complexes with substrate (dUTP), product (dUMP) or inhibitor (dUDP) bound. The native enzyme has been refined at 1.40 A resolution in a hexagonal crystal form and at 2.3 A resolution in an orthorhombic crystal form. In the dUDP complex in a cubic crystal form refined at 2.5 A resolution, the C-terminal conserved P-loop motif is fully ordered. The analysis defines the roles of five sequence motifs in interaction with uracil, deoxyribose and the alpha-, beta- and gamma-phosphates. The enzyme utilizes adaptive recognition to bind the alpha- and beta-phosphates. In particular, the alpha-beta phosphodiester adopts an unfavorable eclipsed conformation in the presence of the P-loop. This conformation may be relevant to the mechanism of alpha-beta phosphodiester bond cleavage.

L60 ANSWER 11 OF 22 MEDLINE on STN
ACCESSION NUMBER: 2001032015 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 10849752
TITLE: Development and validation of homology models of human cathepsins K, S, H, and F.
AUTHOR: Fengler A; Brandt W
CORPORATE SOURCE: Department of Biochemistry and Biotechnology, Martin Luther University Halle-Wittenberg, Saale, Germany.
SOURCE: Advances in experimental medicine and biology, (2000) 477 255-60.
Journal code: 0121103. ISSN: 0065-2598.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200011
ENTRY DATE: Entered STN: 20010322
Last Updated on STN: 20010322
Entered Medline: 20001120

AB Models of the tertiary structures of cathepsins K, S, H, and F were constructed by using homology protein modelling methods and refinements by interactive graphics and energy minimisation. The predicted structures yield information regarding their substrate binding sites and indicate the residues surrounding these sites. The ligand binding sites were characterised and compared with each other by means of calculated molecular electrostatic surface potentials. This will allow designing and development of new ligands specific for these cathepsins in future investigations.

L60 ANSWER 12 OF 22 MEDLINE on STN
ACCESSION NUMBER: 2000114458 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 10651036
TITLE: Structural studies of FIV and HIV-1 proteases complexed with an efficient inhibitor of FIV protease.
AUTHOR: Li M; Morris G M; Lee T; Laco G S; Wong C H; Olson A J; Elder J H; Wlodawer A; Gustchina A
CORPORATE SOURCE: Macromolecular Structure Laboratory, ABL-Basic Research Program, NCI-Frederick Cancer Research and Development Center, Maryland 21702, USA.
CONTRACT NUMBER: P01GM48870 (NIGMS)
R01AI40882 (NIAID)
SOURCE: Proteins, (2000 Jan 1) 38 (1) 29-40.
Journal code: 8700181. ISSN: 0887-3585.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals; AIDS
ENTRY MONTH: 200002
ENTRY DATE: Entered STN: 20000309
Last Updated on STN: 20000309
Entered Medline: 20000224

AB Three forms of feline immunodeficiency virus protease (FIV PR), the wild type (wt) and two single point mutants, V59I and Q99V, as well as human immunodeficiency virus type 1 protease (HIV-1 PR), were cocrystallized with the C2-symmetric inhibitor, TL-3. The mutants of FIV PR were designed to replace residues involved in enzyme-ligand interactions by the corresponding HIV-1 PR residues at the structurally equivalent position. TL-3 shows decreased (improved) inhibition constants with these FIV PR mutants relative to wt FIV PR. Despite similar modes of binding of the inhibitor to all PRs (from P3 to P3'), small differences are evident in the conformation of the Phe side chains of TL-3 at the P1 and P1' positions in the complexes with the mutated FIV PRs. The differences mimick the observed binding of TL-3 in HIV-1 PR and correlate with a significant improvement in the inhibition constants of TL-3 with the two mutant FIV PRs. Large differences between the HIV-1 and FIV PR complexes are evident in the binding modes of the carboxybenzyl groups of TL-3 at P4 and P4'. In HIV-1 PR:TL-3, these groups bind over the flap region, whereas in the FIV PR complexes , the rings are located along the major axis of the active site. A significant difference in the location of the flaps in this region of the HIV-1 and FIV PRs correlates with the observed conformational changes in the binding mode of the peptidomimetic inhibitor at the P4 and P4' positions. These findings provide a structural explanation of the observed Ki values for TL-3 with the different PRs and will further assist in the development of improved inhibitors.

L60 ANSWER 13 OF 22 MEDLINE on STN
ACCESSION NUMBER: 1999146897 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 10022822
TITLE: Crystal structure of MHC class II-associated p41 Ii fragment bound to cathepsin L reveals the structural basis for differentiation between cathepsins L and S.
AUTHOR: Guncar G; Pungercic G; Klemencic I; Turk V; Turk D
CORPORATE SOURCE: Department of Biochemistry and Molecular Biology, Jozcaronef Stefan Institute, Jamova 39, SLO-1000 Ljubljana, Slovenia.
SOURCE: EMBO journal, (1999 Feb 15) 18 (4) 793-803.
Journal code: 8208664. ISSN: 0261-4189.
PUB. COUNTRY: ENGLAND: United Kingdom
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199904
ENTRY DATE: Entered STN: 19990511
Last Updated on STN: 20020420
Entered Medline: 19990426

AB The lysosomal cysteine proteases cathepsins S and L play crucial roles in the degradation of the invariant chain during maturation of MHC class II molecules and antigen processing. The p41 form of the invariant chain includes a fragment which specifically inhibits cathepsin L but not S. The crystal structure of the p41 fragment, a homologue of the thyroglobulin type-1 domains, has been determined at 2.0 A resolution in complex with cathepsin L. The structure of the p41 fragment demonstrates a novel fold, consisting of

two subdomains, each stabilized by disulfide bridges. The first subdomain is an alpha-helix-beta-strand arrangement, whereas the second subdomain has a predominantly beta-strand arrangement. The wedge shape and three-loop arrangement of the p41 fragment bound to the active site cleft of cathepsin L are reminiscent of the inhibitory edge of cystatins, thus demonstrating the first example of convergent evolution observed in cysteine protease inhibitors. However, the different fold of the p41 fragment results in additional contacts with the top of the R-domain of the enzymes, which defines the specificity-determining S2 and S1' substrate-binding sites. This enables inhibitors based on the thyroglobulin type-1 domain fold, in contrast to the rather non-selective cystatins, to exhibit specificity for their target enzymes.

L60 ANSWER 14 OF 22 MEDLINE on STN
ACCESSION NUMBER: 1999096953 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 9878436
TITLE: Crystal structure of dUTPase from equine infectious anaemia virus; active site metal binding in a substrate analogue complex.
AUTHOR: Dauter Z; Persson R; Rosengren A M; Nyman P O; Wilson K S; Cedergren-Zeppezauer E S
CORPORATE SOURCE: Department of Chemistry, University of York, Heslington, YO1 5DD, UK.
SOURCE: Journal of molecular biology, (1999 Jan 15) 285 (2) 655-73.
Journal code: 2985088R. ISSN: 0022-2836.
PUB. COUNTRY: ENGLAND: United Kingdom
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
OTHER SOURCE: PDB-1DUC; PDB-1DUD; PDB-1DUN; PDB-1DUP; PDB-1DUT; PDB-1RDUCSF; PDB-1RDUNSF
ENTRY MONTH: 199903
ENTRY DATE: Entered STN: 19990324
Last Updated on STN: 19990324
Entered Medline: 19990311

AB The X-ray structures of dUTPase from equine infectious anaemia virus (EIAV) in unliganded and complexed forms have been determined to 1.9 and 2.0 A resolution, respectively. The structures were solved by molecular replacement using Escherichia coli dUTPase as search model. The exploitation of a relatively novel refinement approach for the initial model, combining maximum likelihood refinement with stereochemically unrestrained updating of the model, proved to be of crucial importance and should be of general relevance.EIAV dUTPase is a homotrimer where each subunit folds into a twisted antiparallel beta-barrel with the N and C-terminal portions interacting with adjacent subunits. The C-terminal 14 and 17 amino acid residues are disordered in the crystal structure of the unliganded and complexed enzyme, respectively. Interactions along the 3-fold axis include a water-containing volume (size 207 A3) which has no contact with bulk solvent.It has earlier been shown that a divalent metal ion is essential for catalysis. For the first time, a putative binding site for such a metal ion, in this case Sr2+, is established. The positions of the inhibitor (the non-hydrolysable substrate analogue dUDP) and the metal ion in the complex are consistent with the location of the active centre established for trimeric dUTPase structures, in which subunit interfaces form three surface clefts lined with evolutionary conserved residues. However, a detailed comparison of the active sites of the EIAV and E. coli enzymes reveals some structural differences. The viral enzyme undergoes a small conformational change in the uracil-binding beta-hairpin structure upon dUDP binding not observed in the other known dUTPase structures.

L60 ANSWER 15 OF 22 EMBASE COPYRIGHT (c) 2006 Elsevier B.V. All rights reserved on STN
ACCESSION NUMBER: 1999239346 EMBASE Full-text
TITLE: The lysosomal cysteine proteases.
AUTHOR: McGrath M.E.
CORPORATE SOURCE: M.E. McGrath, Axys Pharmaceuticals, Inc., South San Francisco, CA 94080, United States
SOURCE: Annual Review of Biophysics and Biomolecular Structure, (1999) Vol. 28, pp. 181-204.
Refs: 112
ISSN: 1056-8700 CODEN: ABBSE4
COUNTRY: United States
DOCUMENT TYPE: Journal; Article
FILE SEGMENT: 029 Clinical Biochemistry

LANGUAGE: English
SUMMARY LANGUAGE: English
ENTRY DATE: Entered STN: 19990727
Last Updated on STN: 19990727

AB A significant number of exciting papain-like cysteine protease structures have been determined by crystallographic methods over the last several years. This trove of data allows for an analysis of the structural features that empower these molecules as they efficiently carry out their specialized tasks. Although the structure of the paradigm for the family, papain, has been known for twenty years, recent efforts have reaped several structures of specialized mammalian enzymes. This review first covers the commonalities of architecture and purpose of the papain-like cysteine proteases. From that broad platform, each of the lysosomal enzymes for which there is an X-ray structure (or structures) is then examined to gain an understanding of what structural features are used to customize specificity and activity. Structure-based design of inhibitors to control pathological cysteine protease activity will also be addressed.

L60 ANSWER 16 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:546547 CAPLUS Full-text
DOCUMENT NUMBER: 129:272204
TITLE: Use of X-ray Co-crystal Structures and Molecular Modeling To Design Potent and Selective Non-peptide Inhibitors of Cathepsin K
AUTHOR(S): DesJarlais, Renee L.; Yamashita, Dennis S.; Oh, Hye-Ja; Uzinskas, Irene N.; Erhard, Karl F.; Allen, Andrew C.; Haltiwanger, R. Curtis; Zhao, Baoguang; Smith, Ward W.; Abdel-Meguid, Sherin S.; D'Alessio, Karla; Janson, Cheryl A.; McQueney, Michael S.; Tomaszek, Thaddeus A.; Levy, Mark A.; Veber, Daniel F.
CORPORATE SOURCE: Departments of Physical and Structural Chemistry Medicinal Chemistry Analytical Chemistry Structural Biology Protein Biochemistry and Molecular Recognition, SmithKline Beecham Pharmaceuticals, King of Prussia, PA, 19406, USA
SOURCE: Journal of the American Chemical Society (1998), 120(35), 9114-9115
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB By making use of X-ray crystal structures of cathepsin K/inhibitor complexes and mol. modeling, cathepsin K inhibitors of the 1,3-bis(acylamino)-2- propanone series that lack a leucinyl group have now been designed. These inhibitors are equipotent with their closest leucine-derived analogs and are selective for human cathepsin K over human cathepsins B, L, and S. To decrease the peptidic nature of our lead compound, 1,3- bis(Cbz-Leu-NH)-2-propanone 1 analogs were synthesized in which one of the Cbz-Leu groups was replaced with peptidomimetics. For instance, the 2-pyridylsulfonyl analog 2 was notable since it had increased water solubility with only a 2-fold loss in potency relative to 1. Examination of the 3-dimensional structures of cathepsin K/inhibitor complexes, obtained by X-ray crystallog., indicated several important recognition elements in our cathepsin K inhibitors including the iso-Bu side chain of the leucine, which binds in the hydrophobic S23 pocket of the enzyme and the two Cbz Ph rings, which each form aromatic-aromatic interactions, one with Tyr 67 on the unprime side and the other with Trp 184 on the prime3 side of the active site.

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L60 ANSWER 17 OF 22 MEDLINE on STN
ACCESSION NUMBER: 1998318038 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 9655332
TITLE: Crystal structure of human cathepsin S.
AUTHOR: McGrath M E; Palmer J T; Bromme D; Somoza J R
CORPORATE SOURCE: Axys Pharmaceuticals, Inc., South San Francisco, California 94080, USA.. mcgrath@arris.com
SOURCE: Protein science : a publication of the Protein Society, (1998 Jun) 7 (6) 1294-302.
Journal code: 9211750. ISSN: 0961-8368.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English

FILE SEGMENT: Priority Journals
ENTRY MONTH: 199809
ENTRY DATE: Entered STN: 19980910
Last Updated on STN: 19980910
Entered Medline: 19980901

AB We have determined the 2.5 A structure (Rcryst = 20.5%, Rfree = 28.5%) of a complex between human cathepsin S and the potent, irreversible inhibitor 4-morpholinecarbonyl-Phe-hPhe-vinyl sulfone-phenyl. Noncrystallographic symmetry averaging and other density modification techniques were used to improve electron density maps which were nonoptimal due to systematically incomplete data. Methods that reduce the number of parameters were implemented for refinement. The refined structure shows cathepsin S to be similar to related cysteine proteases such as papain and cathepsins K and L. As expected, the covalently-bound inhibitor is attached to the enzyme at Cys 25, and enzyme binding subsites S3-S1' are occupied by the respective inhibitor substituents. A somewhat larger S2 pocket than what is found in similar enzymes is consistent with the broader specificity of cathepsin S at this site, while Lys 61 in the S3 site may offer opportunities for selective inhibition of this enzyme. The presence of Arg 137 in the S1' pocket, and proximal to Cys 25 may have implications not only for substrate specificity C-terminal to the scissile bond, but also for catalysis.

L60 ANSWER 18 OF 22 BIOSIS COPYRIGHT (c) 2006 The Thomson Corporation on STN
ACCESSION NUMBER: 1996:460703 BIOSIS Full-text
DOCUMENT NUMBER: PREV199699183059
TITLE: Active site mutants of pig citrate synthase: Effects of mutations on the enzyme catalytic and structural properties.
AUTHOR(S): Evans, Claudia T.; Kurz, Linda C.; Remington, S. James; Srere, Paul A. [Reprint author]
CORPORATE SOURCE: Dep. Veterans Affairs Med. Cent., Univ. Texas Southwestern Med. Cent. Dallas, Dallas, TX, USA
SOURCE: Biochemistry, (1996) Vol. 35, No. 33, pp. 10661-10672.
CODEN: BICHAW. ISSN: 0006-2960.
DOCUMENT TYPE: Article
LANGUAGE: English
ENTRY DATE: Entered STN: 11 Oct 1996
Last Updated on STN: 11 Oct 1996

AB We examined the catalytic efficiency of 18 pig citrate synthase mutants. The residues mutated were selected according to two criteria: the conservation of that residue in all known citrate synthase sequences, and the importance of that residue in substrate-amino acid interactions suggested by the extensive crystal structure information on the enzyme and its complexes. Several changes were made at certain residues to probe the effects of size, hydrogen bonding, and charge on the kinetics of the enzyme. The mutations, as expected, affected the k- cats and K-ms for OAA and acetyl-CoA to varying degrees. The catalytic efficiency of each of the mutants was determined by the k-cat/K-m for the individual substrates, OAA and acetyl-CoA. All mutations affected kat. There was only one mutant, Asp327Asn, in which the K-ms primarily were affected. Most mutations affected both k-cat and K-m and included the following: His274Gly, His274Arg, Asp375Gly, Asp375Asn, Asp375Glu, Asp375Gln, His320Gly, His320Gln, His320Asn, His320Arg, Arg401His, Gly275Val, and Gly275Ala. The mutations, Arg401Gly, Arg401Lys, His235Gln, and Asn242Glu, had smaller effects on k-cat and K-m. The CS mutant Arg401Lys exhibited a modestly improved k-cat/K-m for both substrates compared to the nonmutant enzyme. X-ray crystallographic studies at 2.7 ANG resolution of one of the mutants, His274Gly, have been undertaken. The mutant enzyme crystallizes in an "open" conformation essentially isomorphous to wild type. The refined model has good geometry and a crystallographic R factor of 0. 187 for 11 441 reflections observed between 6.0 and 2.7 ANG resolution. The refined model revealed a localized relaxation of the structure to relieve strain imposed by a high-energy main and side chain conformation of His274 in the nonmutant, but otherwise the mutation does not result in major structural alterations. Preliminary electrostatic calculations provide support for the concept that the transition state in the rate-limiting step of the citrate synthase catalyzed reaction may be an "enolized" version of acetyl-CoA that is neither neutral nor fully negatively charged and that a possible role for the catalytically essential His274 is to stabilize this by charge delocalization mediated by a hydrogen bond. These results provide the basis for further studies of the effects of these changes on the several reactive intermediates, activated substrates, and transition states which may occur along the reaction coordinate for this type of Claisen enzyme.

L60 ANSWER 19 OF 22 MEDLINE on STN
ACCESSION NUMBER: 94076361 MEDLINE Full-text

DOCUMENT NUMBER: PubMed ID: 8254683
TITLE: Preliminary crystallographic study of a complex between an Fab of a monoclonal feline peritonitis virus neutralizing antibody and its anti-idiotypic Fab.
AUTHOR: Ban N; Escobar C; Day J; Greenwood A; McPherson A
CORPORATE SOURCE: Department of Biochemistry, University of California at Riverside 92521.
CONTRACT NUMBER: GM40706-03 (NIGMS)
SOURCE: Journal of molecular biology, (1993 Dec 5) 234 (3) 894-6.
Journal code: 2985088R. ISSN: 0022-2836.
PUB. COUNTRY: ENGLAND: United Kingdom
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199401
ENTRY DATE: Entered STN: 19940203
Last Updated on STN: 19940203
Entered Medline: 19940112

AB A complex between an Fab fragment of an E2 specific feline infectious peritonitis virus neutralizing antibody 730.1.4 and Fab fragment from anti-idiotypic monoclonal antibody 409.5.3, was crystallized from ammonium sulfate using vapor diffusion methods. The complex crystals diffract to about 2.9 A resolution and are of orthorhombic space group P2(1)22(1) with a = 75.2 A, b = 80.6 A and c = 187.6 A. There are two Fab molecules, or one idiotype-anti-idiotype complex, comprising the asymmetric unit. The long 187.6 A c axis suggests that the long axis of the complex might lie along this direction. Although small and radiation-sensitive, crystals are suitable for three-dimensional structural analysis.

L60 ANSWER 20 OF 22 MEDLINE on STN
ACCESSION NUMBER: 93233116 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 8474099
TITLE: Verapamil analogues with restricted molecular flexibility: synthesis and pharmacological evaluation of the four isomers of alpha-[1-[3-[N-[1- [2-(3,4-dimethoxyphenyl)ethyl]]-N-methylamino]cyclohexyl]]-alpha-isopropyl-3,4-dimethoxybenzene-acetonitrile.
AUTHOR: Dei S; Romanelli M N; Scapecchi S; Teodori E; Gualtieri F; Chiarini A; Voigt W; Lemoine H
CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche, Universita di Firenze, Italy.
SOURCE: Journal of medicinal chemistry, (1993 Feb 19) 36 (4) 439-45.
Journal code: 9716531. ISSN: 0022-2623.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199305
ENTRY DATE: Entered STN: 19930604
Last Updated on STN: 19930604
Entered Medline: 19930519

AB The synthesis and pharmacological activities of the four isomeric racemates of alpha-[1-[3-[N-[1-[2-(3,4-dimethoxyphenyl)ethyl]]-N- methylamino]cyclohexyl]]-alpha-isopropyl-3,4-dimethoxybenzene-acetoni trile are reported (2a-d). The compounds are verapamil analogues with restricted molecular flexibility designed to gather information on the active conformation(s) of the parent drug. The relative stereochemistry of the four racemates was established by X-ray crystallography and by 1H NMR spectroscopy; conformational analysis was supported by theoretical calculations. Negative inotropic and chronotropic activities were evaluated on guinea pig atria, while vasodilatory activity on smooth muscle was tested on guinea pig aortic strips. Binding studies on cat ventricles were performed using (-)-[N-methyl-3H]desmethoxyverapamil (D888) as a reference ligand . The results seem to support the hypothesis that cardiac depressant and vasorelaxant activities are due to different conformations of the verapamil molecule.

L60 ANSWER 21 OF 22 MEDLINE on STN
ACCESSION NUMBER: 88139327 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 3343232
TITLE: Domain interaction in rabbit muscle pyruvate kinase. I. Effects of ligands on protein denaturation

induced by guanidine hydrochloride.
AUTHOR: Consler T G; Lee J C
CORPORATE SOURCE: E. A. Doisy Department of Biochemistry, St. Louis University School of Medicine, Missouri 63104.
SOURCE: Journal of biological chemistry, (1988 Feb 25) 263 (6) 2787-93.
Journal code: 2985121R. ISSN: 0021-9258.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 198803
ENTRY DATE: Entered STN: 19900308
Last Updated on STN: 19980206
Entered Medline: 19880325

AB The structural stability of rabbit muscle pyruvate kinase was examined. The unfolding of pyruvate kinase was induced by guanidine hydrochloride, and the process was monitored by spectroscopic techniques (fluorescence and UV absorption) and hydrodynamic measurements (sedimentation velocity, sedimentation equilibrium, densimetry, and viscometry). The spectroscopic techniques revealed that the unfolding of pyruvate kinase induced by guanidine hydrochloride is not a simple cooperative process. This suggests that different regions of pyruvate kinase are unfolding with different efficiencies in response to the denaturant. These regions are most likely related to the domain structures observed by x-ray crystallography. In the presence of L-phenylalanine, the allosteric inhibitor, the denaturation process became more cooperative, and the enzyme dissociated and unfolded at a higher denaturant concentration. The binding of phenylalanine also induced a structural change in the enzyme, rendering it more susceptible to tryptic digestion. One of the peptides, the production rate of which was increased, was isolated and sequenced. Its N terminus is located at the interface between two domains, one of which contains the active site. This evidence indicates structural changes, probably involving domain-domain interaction, for pyruvate kinase in response to phenylalanine binding.

L60 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1960:17454 CAPLUS Full-text
DOCUMENT NUMBER: 54:17454
ORIGINAL REFERENCE NO.: 54:3565c-f
TITLE: The biochemistry of the eye related to its optical properties
AUTHOR(S): Pirie, Antoinette
CORPORATE SOURCE: Univ. Oxford, UK
SOURCE: Endeavour (1958), 17, 181-9
CODEN: ENDEAS; ISSN: 0160-9327
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB The biochemistry of the eye is interpreted in relation to its transmission of light rather than its reception of light. The transparency of the cornea and lens depend upon their metabolism, especially respiration of the cells. Eye disturbances in galactosemia are discussed. Exptl. cataracts can be produced in young rats in a few days by feeding excessive amts. of galactose or xylose. Delayed biochem. changes resulting from exposure to x-rays are described. Very striking biochem. differences exist in the eyes of different species of vertebrates and even of mammals. The reflection of light by the eyes of cats and dogs at night results from the presence of the tapetum lucidum which acts as a mirror. The crystalline reflecting material in the tapetum lucidum of carnivores is a Zn-cysteine complex. The tapetum lucidum cells of the silver fox contain 16% Zn and 8-9% S on a dry weight basis. Injections of dithizone into dogs abolish reflection by the eyes, followed by blindness. The reflecting material in the eyes of fishes, amphibia, and reptiles is guanine. In the dogfish, Squalus acanthias, the guanine crystals are very large and arranged in a regular way. In dim light they are uncovered, but in bright light they become covered with a pigment. In herbivores (cattle and sheep) the tapetum lucidum consists of fine parallel fibers which reflect colored light. The choroid contains a high concentration of Ba, which may be as high as 120 mg./100 g. dry weight in the choroid of the cow. It is unknown whether the Ba is connected with the tapetum lucidum. 22 references.

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